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Si aucun titre n'est indiqué se référer à la description.)

Protein crystal comprising the processivity clamp factor of DNA polymerase and a
ligand, and its uses

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PROTEIN CRYSTAL COMPRISING THE PROCESSIVITY CLAMP FACTOR OF DNA POLYMERASE AND A LIGAND, AND ITS USES

5 The present invention relates to a protein crystal comprising the processivity clamp factor of DNA polymerase and a peptide comprising all or part of the processivity clamp factor binding sequence of a processivity clamp factor interacting protein, and its uses, in particular for the screening, the design or the modification of ligands of the processivity clamp factor of DNA polymerase.

10 The presence of lesions on DNA may severely impair its replication and have dramatic consequences on cells survival. Beside the activity of efficient repair processes, which remove most of the lesions from DNA before replication occurs, the replisome is able to cope with replication blocking DNA lesions, thanks to specialized biochemical processes referred to as damaged DNA tolerance pathways. Translesion synthesis (TLS) is one of these mechanisms which requires the incorporation of a
15 nucleotide opposite and past the lesion. Depending on the nature of the incorporated nucleotide relative to the parental sequence, the TLS process is error-free or mutagenic. TLS has recently gained much understanding, with the discovery of specialized DNA polymerases, which are able to replicate through lesions which otherwise impede the
20 progression of DNA polymerases involved in replication. These new polymerases have been found in both prokaryotes and eukaryotes and most of them have been classified in the Y superfamily (Ohmori *et al.*, 2001). In *Escherichia coli*, two such polymerases have been identified, Pol IV (DinB) (Wagner *et al.*, 1999) and Pol V (Tang *et al.*, 1999; Reuven *et al.*, 1999), whereas Pol II polymerase has also been shown to perform TLS,
25 although it belongs to the B family (Napolitano *et al.*, 2000; Becherel *et al.*, 2001; Fuchs *et al.*, 2001). Interestingly, all these three polymerase genes are part of the SOS network and are induced upon the arrest of replication due to the presence of replicase blocking lesions onto DNA.

30 The discovery of translesional polymerases (Ohmori *et al.*, 2001) resulted in a major modification of the molecular model of TLS and resulting lesion induced mutagenesis. The previous model, essentially built on genetic experiments in *E. coli* (Bridges and Woodgates, 1985) suggested that the replicative polymerase stalled at blocking lesions was assisted by SOS induced proteins, whose functions were expected to facilitate the polymerase progression through the lesion by increasing its anchoring

onto modified DNA or by reducing its fidelity either by alteration of the correct nucleotide selection process and/or by inhibition of its proofreading activity. The current new model (Cordonnier *et al.*, 1999) proposes that the blocked replicative polymerase is replaced by one or several TLS polymerases that cooperate at different steps of the translesional process, namely incorporation opposite the lesion and elongation of the lesion terminus, to ensure an efficient bypass of the lesion. These polymerases further dissociate from the DNA substrate and the replicative enzyme resumes its synthesis function.

It was demonstrated that prokaryotic and eukaryotic replicative polymerases (Pol III holoenzyme of *E. coli*, pol C, eukaryotic pol δ and pol ϵ) physically interact with their respective processivity clamp factor, also called sliding clamp. Moreover, all prokaryotic and most eukaryotic TLS polymerases also interact with their processivity clamp factor (Lenne-Samuel *et al.*, 2002; Wagner *et al.*, 2000; Becherel *et al.*, 2002; Haracska *et al.*, 2002; Haracska *et al.*, 2001a; Haracska *et al.*, 2001b). These clamps, which act by increasing the replicative polymerase processivity (Bruck and O'Donnell, 2001), are homodimeric (β of *E. coli*) or homotrimeric (gp45 of T4/RB69 or PCNA in eukaryotes) toroid-shape molecules that are loaded onto DNA near primer-template junctions, by specific clamp loader complexes (e.g. the so-called γ complex in *E. coli* and RFC in eukaryotes). The β and PCNA monomers fold into structurally similar subdomains (3 and 2, respectively), despite a lack of internal homology in their amino acids sequences, so that the ring presents a pseudo-six-fold symmetry. A consensus pentapeptidic sequence, QL(SD)LF, conserved among eubacteria, was identified in most of the β -binding proteins as the motif mediating their connection with the clamp, through hydrophobic interactions (Dalrymple *et al.*, 2001). Similarly, a eukaryotic PCNA (or alternative sliding clamps) consensus binding sequence has been identified. A recent study in *E. coli* demonstrated that the integrity of this motif is absolutely required for the inducible polymerases to perform TLS: Pol IV and Pol II mutant proteins deleted for their β -clamp binding motif retain their polymerase activity, but lose their functions in the TLS process *in vivo*, highlighting the fact that their functional interaction with β is crucial for translesion DNA synthesis and mutagenesis (Becherel *et al.*, 2002; Lenne-Samuel *et al.*, 2002).

The presence of several TLS polymerases within a single organism has remained a puzzling question. Analysis of the TLS process in *E. coli* indicated that, depending on

both the nature of the lesion and the local DNA sequence, one or several TLS polymerases may participate to a single TLS event (Napolitano *et al.*, 2000; Wagner *et al.*, 2002). TLS appears as a complex process where a pool of low fidelity polymerases replace the highly stringent replisome and eventually exchange mutually to accommodate the large variety of DNA lesions and to ensure ultimately the completion of DNA replication. Whether this polymerase switching process is somehow coordinated or simply occurs on the basis of competition between the different TLS polymerases is not yet known.

An object of the invention is to provide a method to obtain ligands of the processivity clamp factor which would impair the interaction between the sliding clamp and its interacting proteins.

Such ligands might be useful for the preparation of drugs for the treatment of bacterial diseases or of proliferative disorders.

The invention follows on from the solving by the Inventors of the structure of a co-crystal obtained between the β clamp of *E. coli* and the 16 residues C-terminal peptide of Pol IV DNA polymerase (P16) of *E. coli* containing its β -binding sequence, from the identification of the peptide binding site on β and from the description of the interactions between P16 and β residues.

The Invention also follows on from the results of experiments carried out by the Inventors showing that P16 competes with Pol IV, but also with the α subunit of the *E. coli* replicative Pol III holoenzyme, for binding to β , thus inhibiting their β dependent polymerase activity.

The present invention relates to a protein crystal comprising the processivity clamp factor of DNA polymerase and a peptide of about 3 to about 30 amino acids, in particular of about 16 amino acids, said peptide comprising all or part of the processivity clamp factor binding sequence of a processivity clamp factor interacting protein, such as prokaryotic Pol I, Pol II, Pol III, Pol IV, Pol V, MutS, ligase I, α subunit of DNA polymerase, UmuD or UmuD', or eukaryotic pol ϵ , pol δ , pol η , pol ι , pol κ .

Other processivity clamp factor interacting proteins are notably described in Tsurimoto *et al.* (1999).

The expression "processivity clamp factor of DNA polymerase" refers to *dnaN* genes products and their functional analogs in prokaryotes, and *PCNA* genes products

and their functional analogs and orthologs in eukaryotes. It can also be referred to as a sliding clamp. It is notably described in Kong *et al.* (1992) and Gulbis *et al.* (1996).

"Pol I", "Pol II", "Pol III", "Pol IV", "Pol V" respectively refer to DNA polymerase I, II, III, IV and V, in bacteria, such as *E. coli*, as reviewed in Friedberg *et al.* (2000a), and Friedberg *et al.* (2000b).

"MutS" refers to the product of the *mutS* gene in *E. coli*, and functional analogs and orthologs thereof, involved in mismatch repair.

"Ligase I" refers to the product of the *lig* gene in *E. coli*, and functional analogs and orthologs thereof.

" α subunit of DNA polymerase" refers to the product of the *dnaE* gene in *E. coli*, and functional analogs and orthologs thereof.

"UmuD" refers to the product of the *umuD* gene in *E. coli*, and functional analogs and orthologs thereof.

"Pol ϵ ", "pol δ ", "pol η ", "pol ι ", "pol κ " refer to eukaryotic polymerases as reviewed in Friedberg *et al.* (2000a), and Friedberg *et al.* (2000b).

The invention more particularly relates to a protein crystal as defined above, wherein the processivity clamp factor of DNA polymerase is the β subunit of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, and the peptide has the following sequence:

VTLLDPQMERQLVLGL (SEQ ID NO: 1)

The β subunit of DNA polymerase III of *Escherichia coli* is in particular described in Kong *et al.* (1992).

The invention more particularly relates to a protein crystal as defined above, comprising the β subunit of DNA polymerase III of *Escherichia coli* and the peptide of SEQ ID NO: 1, said crystal belonging to the triclinic space group P1 and its cell dimensions being approximately $a = 41.23 \text{ \AA}$, $b = 65.22 \text{ \AA}$, $c = 73.38 \text{ \AA}$, $\alpha = 73.11^\circ$, $\beta = 85.58^\circ$, $\gamma = 85.80^\circ$.

The expression "triclinic space group P1" refers to a nomenclature well known to the man skilled in the art, it is in particular described in "International tables for X-ray crystallography", Vol. 1 (The Kynoch press, Birmingham, England, 1968)

The expression "cell dimensions" refers to the geometrical description of the smallest volume being repeated in the three dimensions to build the crystal.

The invention more particularly relates to a protein crystal as defined above, characterized by the atomic coordinates such as obtained by the X-ray diffraction of said crystal, said atomic coordinates being represented in Figure 1.

The expression "atomic coordinates" refers to the three coordinates X, Y, Z (given in Å, $1\text{Å}=10^{-10}\text{ m}$) necessary to describe the exact position of each atom in the molecule.

The expression "X-ray diffraction" refers to the phenomenon following which X-rays are scattered in a specific way by a crystal.

Two major X-ray sources can be used: a rotating anode, which is a usual laboratory equipment and/or a synchrotron which is a large-scale equipment, such as the European Synchrotron Radiation Facility (ESRF) in Grenoble, France.

The general methodology to obtain atomic coordinates from X-ray diffraction of a crystal is well known to man skilled in the art, briefly it consists in measuring the intensities of the numerous secondary X-rays beams resulting from the diffraction by the crystal of an incident X-ray beam.

The invention more particularly relates to a protein crystal as defined above, characterized by the atomic coordinates representing the peptide and the peptide binding site of the β subunit of DNA polymerase III of *Escherichia coli*, and being as follows:

ATOM	4045	N	LEU B 155	5.874	17.816	22.109	1.00	1.00	B
ATOM	4046	CA	LEU B 155	6.029	16.359	22.087	1.00	1.00	B
ATOM	4047	CB	LEU B 155	5.055	15.686	23.064	1.00	1.00	B
ATOM	4048	CG	LEU B 155	5.260	16.046	24.536	1.00	1.00	B
ATOM	4049	CD1	LEU B 155	4.256	15.237	25.360	1.00	1.00	B
ATOM	4050	CD2	LEU B 155	6.686	15.757	24.980	1.00	1.00	B
ATOM	4051	C	LEU B 155	5.808	15.776	20.682	1.00	1.00	B
ATOM	4052	O	LEU B 155	6.177	14.613	20.431	1.00	1.00	B
ATOM	4177	N	THR B 172	9.112	11.246	22.902	1.00	1.00	B
ATOM	4178	CA	THR B 172	8.212	10.730	23.917	1.00	1.00	B
ATOM	4179	CB	THR B 172	8.776	11.014	25.344	1.00	1.00	B
ATOM	4180	CG1	THR B 172	7.931	10.400	26.328	1.00	1.00	B
ATOM	4181	CG2	THR B 172	8.870	12.532	25.619	1.00	1.00	B
ATOM	4182	C	THR B 172	6.805	11.269	23.709	1.00	1.00	B
ATOM	4183	O	THR B 172	6.588	12.352	23.145	1.00	1.00	B
ATOM	4192	N	GLY B 174	4.562	10.770	26.397	1.00	1.00	B
ATOM	4193	CA	GLY B 174	3.992	10.745	27.737	1.00	1.00	B
ATOM	4194	C	GLY B 174	3.762	9.337	28.266	1.00	1.00	B
ATOM	4195	O	GLY B 174	3.667	9.141	29.489	1.00	1.00	B
ATOM	4196	N	HIS B 175	3.650	8.349	27.375	1.00	1.00	B
ATOM	4197	CA	HIS B 175	3.440	6.953	27.796	1.00	1.00	B
ATOM	4198	CB	HIS B 175	2.313	6.309	26.977	1.00	1.00	B
ATOM	4199	CG	HIS B 175	0.992	6.997	27.119	1.00	1.00	B
ATOM	4200	CD2	HIS B 175	0.106	7.435	26.193	1.00	1.00	B
ATOM	4201	ND1	HIS B 175	0.420	7.255	28.345	1.00	1.00	B
ATOM	4202	CE1	HIS B 175	-0.763	7.817	28.170	1.00	1.00	B
ATOM	4203	NE2	HIS B 175	-0.977	7.938	26.875	1.00	1.00	B
ATOM	4204	C	HIS B 175	4.706	6.135	27.641	1.00	1.00	B
ATOM	4205	O	HIS B 175	4.990	5.212	28.403	1.00	1.00	B
ATOM	4207	CA	ARG B 176	6.711	5.768	26.422	1.00	18.30	B
ATOM	4208	CB	ARG B 176	6.575	4.633	25.398	1.00	19.53	B
ATOM	4209	CG	ARG B 176	5.329	5.094	23.954	1.00	22.88	B
ATOM	4210	CD	ARG B 176	4.876	4.888	23.657	1.00	22.11	B
ATOM	4211	NE	ARG B 176	4.435	5.312	22.314	1.00	22.09	B
ATOM	4212	CZ	ARG B 176	4.555	4.591	21.202	1.00	20.17	B
ATOM	4213	NH1	ARG B 176	5.159	3.403	21.213	1.00	17.04	B
ATOM	4214	NH2	ARG B 176	3.914	4.977	20.120	1.00	20.02	B
ATOM	4215	C	ARG B 176	7.684	6.807	25.902	1.00	17.30	B

	ATOM	4216	O	ARG	B	176	7.255	7.860	25.374	1.00	18.10	
	ATOM	4217	N	LEU	B	177	8.957	6.504	26.080	1.00	17.97	B
	ATOM	4218	CA	LEU	B	177	10.049	7.360	25.633	1.00	17.85	B
5	ATOM	4219	CB	LEU	B	177	10.664	8.095	26.827	1.00	18.29	B
	ATOM	4220	CG	LEU	B	177	11.921	8.955	26.611	1.00	16.28	B
	ATOM	4221	CD1	LEU	B	177	11.819	10.163	27.559	1.00	19.52	B
	ATOM	4222	CD2	LEU	B	177	13.191	8.172	26.839	1.00	19.12	B
	ATOM	4223	C	LEU	B	177	11.110	6.517	24.964	1.00	18.45	B
10	ATOM	4224	O	LEU	B	177	11.291	5.329	25.281	1.00	18.33	B
	ATOM	4710	N	PRO	B	242	11.254	17.279	27.890	1.00	1.00	B
	ATOM	4711	CD	PRO	B	242	9.987	16.826	27.286	1.00	1.00	B
	ATOM	4712	CA	PRO	B	242	11.660	16.404	28.997	1.00	1.00	B
	ATOM	4713	CB	PRO	B	242	10.688	15.230	28.874	1.00	1.00	B
15	ATOM	4714	CG	PRO	B	242	9.448	15.869	28.336	1.00	1.00	B
	ATOM	4715	C	PRO	B	242	13.124	15.947	28.987	1.00	1.00	B
	ATOM	4716	O	PRO	B	242	13.728	15.748	27.925	1.00	1.00	B
	ATOM	4748	N	ARG	B	246	16.133	11.840	33.560	1.00	1.00	B
	ATOM	4749	CA	ARG	B	246	15.239	11.808	34.707	1.00	1.00	B
20	ATOM	4750	CB	ARG	B	246	14.755	13.227	34.984	1.00	1.00	B
	ATOM	4751	CG	ARG	B	246	15.880	14.252	35.113	1.00	1.00	B
	ATOM	4752	CD	ARG	B	246	16.443	14.295	36.529	1.00	1.00	B
	ATOM	4753	NE	ARG	B	246	15.374	14.318	37.524	1.00	1.00	B
	ATOM	4754	CZ	ARG	B	246	14.316	15.126	37.477	1.00	1.00	B
25	ATOM	4755	NH1	ARG	B	246	14.169	15.992	36.481	1.00	1.00	B
	ATOM	4756	NH2	ARG	B	246	13.396	15.067	38.430	1.00	1.00	B
	ATOM	4757	C	ARG	B	246	14.022	10.889	34.566	1.00	1.00	B
	ATOM	4758	O	ARG	B	246	13.384	10.536	35.560	1.00	1.00	B
	ATOM	4759	N	VAL	B	247	13.695	10.532	33.327	1.00	1.00	B
30	ATOM	4760	CA	VAL	B	247	12.553	9.675	33.018	1.00	1.00	B
	ATOM	4761	CB	VAL	B	247	12.061	9.942	31.585	1.00	1.00	B
	ATOM	4762	CG1	VAL	B	247	10.930	8.991	31.216	1.00	1.00	B
	ATOM	4763	CG2	VAL	B	247	11.624	11.391	31.462	1.00	1.00	B
	ATOM	4764	C	VAL	B	247	12.962	8.218	33.133	1.00	1.00	B
35	ATOM	4765	O	VAL	B	247	12.125	7.334	33.308	1.00	1.00	B
	ATOM	4996	N	PHE	B	278	-7.702	-1.352	24.244	1.00	1.00	B
	ATOM	4997	CA	PHE	B	278	-6.698	-1.155	25.300	1.00	1.00	B
	ATOM	4998	CB	PHE	B	278	-7.318	-1.432	26.663	1.00	1.00	B
40	ATOM	4999	CG	PHE	B	278	-8.431	-0.459	27.021	1.00	1.00	B
	ATOM	5000	CD1	PHE	B	278	-8.142	0.882	27.268	1.00	1.00	B
	ATOM	5001	CD2	PHE	B	278	-9.760	-0.869	27.021	1.00	1.00	B
	ATOM	5002	CE1	PHE	B	278	-9.177	1.816	27.508	1.00	1.00	B
	ATOM	5003	CE2	PHE	B	278	-10.795	0.052	27.258	1.00	1.00	B
	ATOM	5004	CZ	PHE	B	278	-10.496	1.391	27.500	1.00	1.00	B
45	ATOM	5005	C	PHE	B	278	-5.403	-1.957	25.131	1.00	1.00	B
	ATOM	5006	O	PHE	B	278	-4.356	-1.582	25.677	1.00	1.00	B
	ATOM	5332	N	ASN	B	320	0.635	-2.143	27.431	1.00	1.00	B
	ATOM	5333	CA	ASN	B	320	-0.051	-1.983	26.158	1.00	1.00	B
	ATOM	5334	CB	ASN	B	320	-0.055	-0.504	25.796	1.00	1.00	B
50	ATOM	5335	CG	ASN	B	320	-0.561	-0.259	24.407	1.00	1.00	B
	ATOM	5336	OD1	ASN	B	320	-0.226	-0.997	23.481	1.00	1.00	B
	ATOM	5337	ND2	ASN	B	320	-1.362	0.791	24.242	1.00	1.00	B
	ATOM	5338	C	ASN	B	320	0.927	-2.745	25.249	1.00	1.00	B
	ATOM	5339	O	ASN	B	320	2.093	-2.350	25.102	1.00	1.00	B
55	ATOM	5353	N	TYR	B	323	2.932	-0.853	22.482	1.00	1.00	B
	ATOM	5354	CA	TYR	B	323	4.110	-0.088	22.908	1.00	1.00	B
	ATOM	5355	CB	TYR	B	323	3.878	0.590	24.259	1.00	1.00	B
	ATOM	5356	CG	TYR	B	323	2.813	1.668	24.294	1.00	1.00	B
	ATOM	5357	CD1	TYR	B	323	2.397	2.314	23.127	1.00	1.00	B
60	ATOM	5358	CE1	TYR	B	323	1.458	3.374	23.170	1.00	1.00	B
	ATOM	5359	CD2	TYR	B	323	2.284	2.093	25.509	1.00	1.00	B
	ATOM	5360	CE2	TYR	B	323	1.354	3.166	25.567	1.00	1.00	B
	ATOM	5361	CZ	TYR	B	323	0.957	3.790	24.399	1.00	1.00	B
65	ATOM	5362	OH	TYR	B	323	0.112	4.886	24.453	1.00	1.00	B
	ATOM	5363	C	TYR	B	323	5.327	-1.018	23.041	1.00	1.00	B
	ATOM	5364	O	TYR	B	323	6.468	-0.646	22.726	1.00	1.00	B
	ATOM	5519	N	VAL	B	344	3.837	-1.100	39.291	1.00	1.00	B
	ATOM	5520	CA	VAL	B	344	3.324	0.227	39.030	1.00	1.00	B
	ATOM	5521	CB	VAL	B	344	2.676	0.818	40.318	1.00	1.00	B
70	ATOM	5522	CG1	VAL	B	344	1.474	-0.026	40.725	1.00	1.00	B
	ATOM	5523	CG2	VAL	B	344	3.687	0.847	41.456	1.00	1.00	B
	ATOM	5524	C	VAL	B	344	4.405	1.163	38.512	1.00	1.00	B
	ATOM	5525	O	VAL	B	344	4.199	2.365	38.405	1.00	1.00	B
	ATOM	5532	N	SER	B	346	7.618	2.153	35.615	1.00	21.53	B
75	ATOM	5533	CA	SER	B	346	8.060	2.002	34.239	1.00	21.50	B
	ATOM	5534	CB	SER	B	346	8.655	3.320	33.723	1.00	21.47	B
	ATOM	5535	OG	SER	B	346	9.793	3.703	34.474	1.00	26.08	B
	ATOM	5536	C	SER	B	346	9.107	0.914	34.106	1.00	20.70	B

	ATOM	5537	O	SER	B	346	9.755	0.521	35.078	1.00	21.55	
	ATOM	5632	N	VAL	B	360	11.730	3.546	27.545	1.00	1.00	B
	ATOM	5633	CA	VAL	B	360	11.023	3.501	28.812	1.00	1.00	B
5	ATOM	5634	CB	VAL	B	360	11.276	4.794	29.641	1.00	1.00	B
	ATOM	5635	CG1	VAL	B	360	10.448	4.742	30.934	1.00	1.00	B
	ATOM	5636	CG2	VAL	B	360	12.753	4.923	29.937	1.00	1.00	B
	ATOM	5637	C	VAL	B	360	9.562	3.381	28.501	1.00	1.00	B
	ATOM	5638	O	VAL	B	360	9.008	4.188	27.753	1.00	1.00	B
10	ATOM	5639	N	VAL	B	361	8.905	2.372	29.069	1.00	19.72	B
	ATOM	5640	CA	VAL	B	361	7.488	2.188	28.831	1.00	18.92	B
	ATOM	5641	CB	VAL	B	361	7.216	0.872	28.069	1.00	18.99	B
	ATOM	5642	CG1	VAL	B	361	5.743	0.769	27.716	1.00	18.31	B
	ATOM	5643	CG2	VAL	B	361	8.065	0.839	26.786	1.00	17.76	B
15	ATOM	5644	C	VAL	B	361	6.793	2.100	30.167	1.00	19.47	B
	ATOM	5645	O	VAL	B	361	7.232	1.362	31.038	1.00	16.90	B
	ATOM	5646	N	MET	B	362	5.737	2.885	30.318	1.00	1.00	B
	ATOM	5647	CA	MET	B	362	4.962	2.882	31.540	1.00	1.00	B
	ATOM	5648	CB	MET	B	362	4.226	4.206	31.682	1.00	1.00	B
20	ATOM	5649	CG	MET	B	362	3.918	4.589	33.122	1.00	1.00	B
	ATOM	5650	SD	MET	B	362	5.405	4.806	34.163	1.00	1.00	B
	ATOM	5651	CE	MET	B	362	4.575	4.880	35.731	1.00	1.00	B
	ATOM	5652	C	MET	B	362	3.949	1.731	31.471	1.00	1.00	B
	ATOM	5653	O	MET	B	362	3.385	1.438	30.410	1.00	1.00	B
25	ATOM	5654	N	PRO	B	363	3.698	1.069	32.599	1.00	1.00	B
	ATOM	5655	CD	PRO	B	363	4.521	1.025	33.818	1.00	1.00	B
	ATOM	5656	CA	PRO	B	363	2.729	-0.038	32.579	1.00	1.00	B
	ATOM	5657	CB	PRO	B	363	3.155	-0.883	33.776	1.00	1.00	B
	ATOM	5658	CG	PRO	B	363	3.665	0.160	34.754	1.00	1.00	B
30	ATOM	5659	C	PRO	B	363	1.272	0.395	32.672	1.00	1.00	B
	ATOM	5660	O	PRO	B	363	0.959	1.574	32.811	1.00	1.00	B
	ATOM	5661	N	MET	B	364	0.368	-0.568	32.537	1.00	1.00	B
	ATOM	5662	CA	MET	B	364	-1.037	-0.272	32.674	1.00	1.00	B
	ATOM	5663	CB	MET	B	364	-1.780	-0.391	31.332	1.00	1.00	B
35	ATOM	5664	CG	MET	B	364	-1.636	-1.670	30.568	1.00	1.00	B
	ATOM	5665	SD	MET	B	364	-2.386	-1.510	28.872	1.00	1.00	B
	ATOM	5666	CE	MET	B	364	-4.155	-1.253	29.308	1.00	1.00	B
	ATOM	5667	C	MET	B	364	-1.602	-1.218	33.725	1.00	1.00	B
40	ATOM	5668	O	MET	B	364	-0.999	-2.251	34.035	1.00	1.00	B
	ATOM	5669	N	ARG	B	365	-2.732	-0.836	34.307	1.00	1.00	B
	ATOM	5670	CA	ARG	B	365	-3.383	-1.655	35.324	1.00	1.00	B
	ATOM	5671	CB	ARG	B	365	-4.029	-0.756	36.394	1.00	1.00	B
	ATOM	5672	CG	ARG	B	365	-4.785	-1.490	37.505	1.00	1.00	B
45	ATOM	5673	CD	ARG	B	365	-3.859	-2.316	38.398	1.00	1.00	B
	ATOM	5674	NE	ARG	B	365	-4.571	-2.956	39.505	1.00	1.00	B
	ATOM	5675	CZ	ARG	B	365	-3.984	-3.707	40.434	1.00	1.00	B
	ATOM	5676	NH1	ARG	B	365	-2.678	-3.913	40.385	1.00	1.00	B
	ATOM	5677	NH2	ARG	B	365	-4.698	-4.247	41.418	1.00	1.00	B
50	ATOM	5678	C	ARG	B	365	-4.459	-2.492	34.648	1.00	1.00	B
	ATOM	5679	O	ARG	B	365	-5.449	-1.961	34.150	1.00	1.00	B
	ATOM	5680	N	LEU	B	366	-4.267	-3.801	34.609	1.00	41.59	B
	ATOM	5681	CA	LEU	B	366	-5.272	-4.665	33.996	1.00	44.25	B
	ATOM	5682	CB	LEU	B	366	-4.615	-5.908	33.366	1.00	45.24	B
55	ATOM	5683	CG	LEU	B	366	-3.640	-5.701	32.202	1.00	45.46	B
	ATOM	5684	CD1	LEU	B	366	-4.331	-5.029	31.031	1.00	47.09	B
	ATOM	5685	CD2	LEU	B	366	-2.489	-4.856	32.678	1.00	46.71	B
	ATOM	5686	C	LEU	B	366	-6.263	-5.080	35.092	1.00	45.55	B
	ATOM	5687	O	LEU	B	366	-6.424	-6.296	35.333	1.00	46.32	B
	ATOM	5688	OXT	LEU	B	366	-6.868	-4.169	35.704	1.00	46.33	B
60	ATOM	5689	CB	ARG	C	10	-5.663	0.205	32.737	0.76	1.00	C
	ATOM	5690	CG	ARG	C	10	-7.073	-0.397	32.771	0.76	1.00	C
	ATOM	5691	CD	ARG	C	10	-7.748	-0.383	31.408	0.76	1.00	C
	ATOM	5692	NE	ARG	C	10	-8.728	-1.462	31.268	0.76	1.00	C
	ATOM	5693	CZ	ARG	C	10	-9.992	-1.301	30.875	0.76	1.00	C
65	ATOM	5694	NH1	ARG	C	10	-10.464	-0.093	30.582	0.76	1.00	C
	ATOM	5695	NH2	ARG	C	10	-10.779	-2.365	30.749	0.76	1.00	C
	ATOM	5696	C	ARG	C	10	-4.106	2.152	32.497	0.76	1.00	C
	ATOM	5697	O	ARG	C	10	-3.278	1.863	33.369	0.76	1.00	C
	ATOM	5698	N	ARG	C	10	-6.417	2.186	31.464	0.76	1.00	C
70	ATOM	5699	CA	ARG	C	10	-5.587	1.727	32.625	0.76	1.00	C
	ATOM	5700	N	GLN	C	11	-3.805	2.853	31.408	0.76	1.00	C
	ATOM	5701	CA	GLN	C	11	-2.458	3.321	31.094	0.76	1.00	C
	ATOM	5702	CB	GLN	C	11	-2.423	3.866	29.662	0.76	1.00	C
	ATOM	5703	CG	GLN	C	11	-1.047	4.361	29.231	0.76	1.00	C
75	ATOM	5704	CD	GLN	C	11	-0.039	3.245	29.174	0.76	1.00	C
	ATOM	5705	OE1	GLN	C	11	-0.263	2.232	28.494	0.76	1.00	C
	ATOM	5706	NE2	GLN	C	11	-1.082	3.415	29.876	0.76	1.00	C
	ATOM	5707	C	GLN	C	11	-1.895	4.396	32.038	0.76	1.00	C

ATOM	5708	O	GLN	C	11	-2.494	5.467	32.217	0.76	1.00	C
ATOM	5709	N	LEU	C	12	-0.732	4.111	32.618	0.76	1.00	C
ATOM	5710	CA	LEU	C	12	-0.065	5.046	33.519	0.76	1.00	C
ATOM	5711	CB	LEU	C	12	0.754	4.277	34.561	0.76	1.00	C
ATOM	5712	CG	LEU	C	12	-0.036	3.305	35.450	0.76	1.00	C
ATOM	5713	CD1	LEU	C	12	0.907	2.681	36.468	0.76	1.00	C
ATOM	5714	CD2	LEU	C	12	-1.184	4.040	36.153	0.76	1.00	C
ATOM	5715	C	LEU	C	12	0.845	5.948	32.680	0.76	1.00	C
ATOM	5716	O	LEU	C	12	1.111	5.653	31.510	0.76	1.00	C
ATOM	5717	N	VAL	C	13	1.317	7.044	33.273	0.76	1.00	C
ATOM	5718	CA	VAL	C	13	2.166	7.987	32.543	0.76	1.00	C
ATOM	5719	CB	VAL	C	13	1.473	9.371	32.386	0.76	1.00	C
ATOM	5720	CG1	VAL	C	13	0.217	9.239	31.523	0.76	1.00	C
ATOM	5721	CG2	VAL	C	13	1.113	9.929	33.750	0.76	1.00	C
ATOM	5722	C	VAL	C	13	3.542	8.211	33.174	0.76	1.00	C
ATOM	5723	O	VAL	C	13	3.740	8.050	34.381	0.76	1.00	C
ATOM	5724	N	LEU	C	14	4.498	8.596	32.339	0.76	1.00	C
ATOM	5725	CA	LEU	C	14	5.860	8.846	32.803	0.76	1.00	C
ATOM	5726	CB	LEU	C	14	6.836	8.819	31.619	0.76	1.00	C
ATOM	5727	CG	LEU	C	14	6.972	7.481	30.889	0.76	1.00	C
ATOM	5728	CD1	LEU	C	14	7.666	7.705	29.557	0.76	1.00	C
ATOM	5729	CD2	LEU	C	14	7.744	6.495	31.769	0.76	1.00	C
ATOM	5730	C	LEU	C	14	6.010	10.186	33.517	0.76	1.00	C
ATOM	5731	O	LEU	C	14	5.238	11.126	33.284	0.76	1.00	C
ATOM	5732	N	GLY	C	15	7.000	10.263	34.396	0.76	1.00	C
ATOM	5733	CA	GLY	C	15	7.264	11.510	35.090	0.76	1.00	C
ATOM	5734	C	GLY	C	15	8.263	12.275	34.234	0.76	1.00	C
ATOM	5735	O	GLY	C	15	9.472	12.210	34.462	0.76	1.00	C
ATOM	5736	N	LEU	C	16	7.750	12.995	33.241	0.76	1.00	C
ATOM	5737	CA	LEU	C	16	8.576	13.756	32.306	0.76	1.00	C
ATOM	5738	CB	LEU	C	16	7.732	14.157	31.094	0.76	1.00	C
ATOM	5739	CG	LEU	C	16	7.258	12.955	30.269	0.76	1.00	C
ATOM	5740	CD1	LEU	C	16	6.303	13.411	29.171	0.76	1.00	C
ATOM	5741	CD2	LEU	C	16	8.467	12.233	29.690	0.76	1.00	C
ATOM	5742	C	LEU	C	16	9.263	14.982	32.898	0.76	1.00	C
ATOM	5743	O	LEU	C	16	10.182	15.515	32.231	0.76	1.00	C
ATOM	5744	OXT	LEU	C	16	8.870	15.398	34.009	0.76	1.00	C
END											

wherein atoms 4045 to 5688 represent the peptide binding site and atoms 5689 to 5748 represent the peptide.

The atomic coordinates are represented in protein data bank (pdb) format. Such a format is well known to the man skilled in the art.

According to another embodiment, the invention relates to a method to purify the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, comprising the following steps:

- elution of a solution containing the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, through a cation exchange column, in particular a SP sepharose column;
- elution of a solution containing the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, in particular as obtained by the preceding step, through an anion exchange column, in particular a Mono Q column;
- elution of a solution containing the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase III of

Escherichia coli, in particular as obtained by the preceding step, through a cation exchange column, in particular a Mono S column.

The expression "purify" relates to the process of separating a protein of interest from substantially all the other components of a solution containing said protein of interest, such as a bacterial extract.

Assessment of the purity of the protein of interest can be carried out by methods well known to the man skilled in the art, such as polyacrylamide gel electrophoresis analysis and Coomassie Blue staining or other type of protein staining (e.g. silver staining), mass spectrometry, protein sequencing, HPLC (high performance liquid chromatography). Quantification can be measured by absorbance spectroscopy, Bradford colorimetric assay, or protein sequencing.

The SP sepharose column, Mono Q column and Mono S column are obtained from Pharmacia (Uppsala, Sweden).

Alternatively, columns carrying ion exchange groups with properties similar to those of the SP sepharose column, Mono Q column and Mono S column can also be used.

The above mentioned column can be used with a FPLC system (Pharmacia), and possesses a high protein binding capacity. Advantageously, the SP sepharose column is used during the initial steps of the purification process because it is usually not clogged by dirty samples. The Mono Q and Mono S column are used during the last steps of the purification process, they are highly resolutive columns, but they are easily clogged by dirty samples.

The invention also relates to a method to obtain a protein crystal as defined above, comprising the following steps:

- mixing a solution of processivity clamp factor of DNA polymerase, with a solution of a peptide of about 3 to about 30 amino acids, in particular of about 16 amino acids, said peptide comprising all or part of the processivity clamp factor binding sequence of a processivity clamp factor interacting protein, such as prokaryotic Pol I, Pol II, Pol III, Pol IV, Pol V, MutS, ligase I, α subunit of DNA polymerase, UmuD or UmuD', or eukaryotic pol ϵ , pol δ , pol η , pol ι , pol κ , and with a solution of MES pH 6.0 0.2 M, CaCl_2 0.2 M, PEG 400 60%, to obtain a crystallisation drop,

- letting the crystallisation drop concentrate against a solution of MES pH 6.0 0.1 M, CaCl₂ 0.1 M, PEG 400 30%, by vapour diffusion, to obtain a protein crystal.

5 The expression "vapour diffusion" refers to a crystallization method for macromolecules well known to the man skilled in the art, it is in particular described in "Crystallization of nucleic acids and proteins", pp. 130-145. A. Ducruix & R. Giegé eds., 1999, Oxford University Press.

MES refers to 2-(N-morpholino)-ethane sulfonic acid.

PEG 400 refers to polyethylene glycol 400.

10 Advantageously MES, PEG and CaCl₂ can be obtained from Hampton Research, (Laguna Niguel, USA).

The invention more particularly relates to a method to obtain a protein crystal as defined above, wherein the processivity clamp factor of DNA polymerase is the β subunit of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, in particular as purified according the abovementioned methods of purification, and the peptide has the following sequence:

VTLLDPQMERQLVLGL (SEQ ID NO: 1).

20 According to a preferred embodiment the β subunit of DNA polymerase III of *Escherichia coli* and the peptide of SEQ ID NO: 1 are mixed in a molar ratio of about 1:1 to about 1:3 in particular about 1: 1.5

According to another preferred embodiment the concentration of the β subunit of DNA polymerase III of *Escherichia coli* is from about 8 mg/ml to about 50 mg/ml, in particular about 34 mg/ml.

25 According to another preferred embodiment the concentration of the peptide of SEQ ID NO: 1 is from about 0.5 mg/ml to about 1.2 mg/ml, in particular about 1.1 mg/ml.

30 According to another embodiment, the invention relates to the use of the atomic coordinates as defined above, for the screening, the design or the modification of ligands of the processivity clamp factor of DNA polymerase, in particular of the β subunit of DNA polymerase III of *Escherichia coli*.

The expression "ligand" refers to a compound which is liable to bind to the processivity clamp factor of DNA polymerase.

The invention also relates to the use as defined above, for the screening, the design or the modification of ligands liable to be used for the preparation of pharmaceutical compositions useful for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or proliferative disorders, such as cancers.

The expression "bacterial diseases" refers to diseases which are caused by bacterial influences, such as infections.

The expression "proliferative disorders" refers to disorders which are linked to abnormal cell multiplication, such as cancers.

The invention also relates to a method to screen ligands of the processivity clamp factor of DNA polymerase, said method comprising the step of assessing the interaction of tridimensional models of the ligands to screen with the structure of the β subunit of DNA polymerase as defined by the atomic coordinates as defined above, and in particular with the structure of the peptide binding site as defined by the atomic coordinates defined above, and more particularly with at least nine of the following amino acids: Leu 155, Thr 172, Gly 174, His 175, Arg 176, Leu 177, Pro 242, Arg 246, Val 247, Phe 278, Asn 320, Tyr 323, Val 344, Ser 346, Val 360, Val 361, Met 362, Pro 363, Met 364, Arg 365, Leu 366.

Assessing the interaction can be done by methods such as molecular dynamics, energy calculation, continuum electrostatics, semi-empirical free energy functions and other related methods well known to the man skilled in the art. Several packages and softwares are available for these purposes such as CHARM, UHBD, or SYBILL.

The invention more particularly relates to a method as defined above, to screen ligands liable to be used for the preparation of pharmaceutical compositions useful for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or proliferative disorders, such as cancers.

The invention also relates to a method to design or to modify compounds liable to bind to the processivity clamp factor of DNA polymerase, said method comprising the step of designing or modifying a compound, so that the tridimensional model of said compound is liable to interact with the structure of the β subunit of DNA polymerase as defined by the atomic coordinates as defined above, and in particular with the structure of the peptide binding site as defined by the atomic coordinates as defined above, and more particularly with at least nine of the following amino acids: Leu 155, Thr 172, Gly

174, His 175, Arg 176, Leu 177, Pro 242, Arg 246, Val 247, Phe 278, Asn 320, Tyr 323, Val 344, Ser 346, Val 360, Val 361, Met 362, Pro 363, Met 364, Arg 365, Leu 366.

The invention more particularly relates to a method as defined above, to design or to modify ligands liable to be used for the preparation of pharmaceutical compositions useful for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or proliferative disorders, such as cancers.

According to another embodiment, the invention relates to a peptide of the following sequence:

VTLLDPQMÈRQLVLGL (SEQ ID NO: 1).

According to a preferred embodiment, said peptide comprises non-hydrolysable bonds between amino-acids and/or non-amide bonds between amino-acids.

The invention also relates to a pharmaceutical composition comprising as active substance the peptide of SEQ ID NO: 1, in association with a pharmaceutically acceptable carrier.

Examples of pharmaceutically acceptable carrier are well known to the man skilled in the art.

According to a preferred embodiment, said peptide comprises non-hydrolysable bonds between amino-acids and/or non-amide bonds between amino-acids.

According to another embodiment the invention relates to the use of the peptide of SEQ ID NO: 1, as an anti-bacterial compound.

The expression "anti-bacterial compound" refers to a compound which has bactericidal or bacteriostatic properties, such as an antibiotic.

According to a preferred embodiment, said peptide comprises non-hydrolysable bonds between amino-acids and/or non-amide bonds between amino-acids.

The invention more particularly relates to the use of the peptide of SEQ ID NO: 1 for the manufacture of a medicament for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or proliferative disorders, such as cancers.

According to another embodiment the invention relates to a method to test *in vitro* the inhibitory effect of compounds on the processivity clamp factor-dependant activity of DNA polymerase, in particular of Pol IV DNA polymerase of *Escherichia coli*, or of the α subunit of Pol III DNA polymerase of *Escherichia coli*, comprising the following steps:

- adding to assay solutions comprising a labelled nucleotidic primer, a template DNA, and DNA polymerase, in particular Pol IV DNA polymerase of *Escherichia coli*, or the α subunit of Pol III DNA polymerase of *Escherichia coli*, a compound to test at a given concentration for each assay solution, in the presence or the absence of the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase in particular the β subunit of DNA polymerase III of *Escherichia coli*,

- electrophoretically migrating the abovementioned assay solutions,

- comparing the migration pattern of each assay solutions in the presence or the absence of the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*.

According to a preferred embodiment the assay solutions also comprise a clamp loader, in particular the γ complex of *E. coli*, adenosine triphosphate (ATP), the divalent cation Mg^{2+} and single strand binding protein (SSB) of *E. coli*.

The invention also relates to the use of the method defined above, for the screening of compounds liable to be used for the preparation of pharmaceutical compositions useful for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or proliferative disorders, such as cancers.

BRIEF DESCRIPTION OF THE FIGURES

Figure 1

Figure 1 represents the atomic coordinates in protein databank (pdb) format of the crystallographic structure of the complex between *Escherichia coli* β subunit of DNA polymerase III and the 16 C-terminal residues of the β binding peptide of *E. coli* Pol IV DNA polymerase (P16)

Figure 2

Figure 2 represents a ribbon representation of the β subunit of DNA polymerase III of *E. coli* complexed with the P16 peptide (boxed) as obtained from the crystallographic structure of the complex.

Figure 3A, Figure 3B, Figure 3C and Figure 3D

Figure 3A and Figure 3B represent the inhibition of β dependant activity of Pol IV by the Pol IV β binding peptide, P16

Figure 3C and Figure 3D represent the inhibition of β dependant activity of Pol III α subunit by the Pol IV β binding peptide, P16.

Figure 3A represents the migration pattern of an electrophoresis gel. β free (lanes 1-4 and 9-12) or β loaded (lanes 5-8 and 13-16) labelled primer/template hybrids are incubated with increasing amounts of control peptide (CLIP) (lanes 1-8) or P16 peptide (lanes 9-16). Concentrations of peptides are as follows: 0 μ M, lanes 1, 5, 9 and 13; 1 μ M, lanes 2, 6, 10 and 14; 10 μ M, lanes 3, 7, 11 and 15; 25 μ M, lanes 4, 8, 12 and 16. This mixture is then submitted to the enzymatic activity of Pol IV (1.5 nM) in the presence of each four dNTPs for 1 minute at room temperature. Beside the overall increase in DNA synthesis activity, the β -dependent activity of the polymerase is characterised by the apparition of synthesis products longer than 12 nucleotides (β dependent synthesis), β independent synthesis is characterised by products shorter than 12 nucleotides. The broader band at the bottom of the gel corresponds to the primer.

Figure 3B represents the quantitative analysis of the relative amounts of each β -independent (incorporation of 1 up to 12 nucleotides) and β -dependent (12 and more nucleotides incorporation) activities observed in lanes 5-8 and 13-16. Black and white rectangles represent the ratio of β -dependent to β -independent polymerase activities

(vertical axis) in the presence of specified amounts of CLIP and P16 peptides (horizontal axis), respectively. Decrease in this ratio value actually indicates a specific inhibition of the β -dependent polymerase activity.

Figure 3C and 3D respectively correspond to the same experiments than those represented in Figure 3A and 3B, except that the polymerase used is the purified α subunit of Pol III (6 nM).

Figure 4

Figure 4 represents the growth rate of *E. coli* transformed by IPTG inducible plasmids expressing either the wild type Pol IV (pWp4) (triangles) or the Pol IVD5 mutant of Pol IV lacking the 5 C-terminal amino-acids (pD5p4) (squares, dotted line) in the presence of IPTG. The vertical axis represents the OD at 600 nm and the horizontal axis the time in minutes.

EXAMPLES

EXAMPLE 1

Crystallographic study of the *Escherichia coli* β sliding clamp complexed with the β binding peptide of Pol IV DNA Polymerase of *E. coli*.

1. β binding peptide synthesis and purification

The 16-mer peptide sequence VTLLDPQMERQLVLGL (P16) (SEQ ID NO: 1), representing the 16 last residues of Pol IV DNA polymerase of *E. coli*, was obtained purified from Neosystem (Illkirch, France) and the 22-mer control peptide RPKVKTTPNGAEDESAAEAPPLEF (CLIP) (SEQ ID NO: 2) was a gift from Dr J.P. Briand (Strasbourg, France). P16 was resuspended at 1.1 mg/ml in a buffer containing Tris HCl 20 mM, pH 7.5, 5 mM EDTA, 20% glycerol, and kept at -80°C . CLIP was resuspended in 20 mM NaHCO_3 buffer, pH 9, at concentrations of 250, 100 and 10 pmoles/ μl

2. β protein purification

The *dnaN* gene encoding *E. coli* β sliding clamp (hereafter referred to as β protein) was cloned into the pET15b plasmid (Invitrogen). The β protein was expressed in a transformed *E. coli* BL21(DE3)pLysS/(pET15b-*dnaN*) and was purified as described (Johanson *et al.*, 1986) with the following modifications. A SP Sepharose column (Pharmacia, Upsalla, Sweden) was used instead of the SP Sephadex column. A Mono Q column (Pharmacia, Upsalla, Sweden) followed by a Mono S column (Pharmacia, Upsalla, Sweden) were performed after the SP Sepharose column step. The β protein was purified to >99% purity, as judged by Coomassie gel analysis, and concentrated using Centriplus YM-30 concentrators (Amicon) to 34.2 mg/ml in a buffer containing 20 mM Tris-HCl pH 7.5, 0.5 mM EDTA and 20% (v/v) glycerol, as determined by Bradford assay, using BSA as a standard.

3. Crystallization conditions

Drops were obtained by mixing 0.92 μL of β protein at 34.2 mg/ml (775 pmoles) with 1.89 μL of P16 at 1.1 mg/ml (1136 pmoles) and 1 μL of 2X reservoir solution. Reservoir solution contains 0.1 M MES pH 6.0, 0.1M CaCl_2 and 30% PEG 400 (Hampton Research, Laguna Niguel, CA, USA). The peptide/ β monomer molar ratio was 1.46. Co-crystals were

grown by vapour diffusion in hanging drops at 20°C. They typically grew within three days and reached $200 \times 100 \times 40 \mu\text{m}^3$. Crystals were mounted in loops (Hampton Research, Laguna Niguel, CA, USA), frozen in liquid ethane and kept in liquid nitrogen before collection of crystallographic data.

5

4. Data collection and structure determination

Diffraction data were collected at beam line ID 14-EH4 (ESRF, Grenoble, France). The data were integrated with DENZO and normalized with SCALEPACK (Z. Otwinowski and W. Minor "Processing of X-ray Diffraction Data Collected in Oscillation Mode", 10 Methods in Enzymology, Volume 276; Macromolecular Crystallography, part A, p. 307-326, 1997, C.W. Carter, Jr. and R.M. Sweet, Eds., Academic Press (New York)). The structure was solved by molecular replacement with MOLREP (CCP4, COLLABORATIVE COMPUTATIONAL PROJECT, NUMBER 4. (1994) "The CCP4 Suite: Programs for Protein Crystallography". Acta Cryst. D50, 760-763.), using the known β protein structure as 15 a search model (Kong *et al.*, 1992). The peptide was built with the graphics program O (Copyright 1990 by Alwyn Jones, DatOno AB, Blueberry Hill, S-75591 Uppsala, Sweden) and the model was refined with O and CNS (Brunger *et al.*, 1998) (Copyright © 1997-2001 Yale University).

The results are summarized in following Table 1:

<u>Data collection</u>	
Space group	P1
Cell parameters	$a=41.23 \text{ \AA}$; $b=65.22 \text{ \AA}$; $c=73.38 \text{ \AA}$; $\alpha=73.11^\circ$; $\beta=85.58^\circ$; $\gamma=85.80^\circ$
X-ray source	ID14eh4
Wavelength (\AA)	0.93922
Asymmetric unit	1 dimer
Resolution (\AA)	1.65
Number of observations	
Unique	85999
Total	231008
Completeness (%)	96.7 (95.4) ^a
Rsym	0.051 (0.254) ^a
Mean I/ σ	15.5 (4.3) ^a

Refinement	
Resolution range (Å)	500-1.65
R-factor, reflections	20.87, 80566
Rfree, reflexions	23.71, 4226
Number of atoms	
Protein	5744
Water	443
R.m.s deviation	
Bond angles (°)	1.59
Bond lengths (Å)	0.013
Average atomic B-value (Å ²)	
Protein	
β	22.8
Peptide	29.7
Water	29.1
Ramachandran plot ^b (%)	
residues in core,	92.4
allowed,	6.9
generously allowed regions	0.8

^a Number in parentheses is for the last shell (1.71-1.65)

^b Statistics from *PROCHECK* (Laskowski *et al.*, 1993)

Table 1: Crystal structure data and refinement statistics

5 The results obtained indicate that the crystal is triclinic, with cell dimensions $a = 41.23$ Å, $b = 65.22$ Å, $c = 73.38$ Å, $\alpha = 73.11^\circ$, $\beta = 85.58^\circ$, $\gamma = 85.79^\circ$. These cell parameters lead to a quite usual value of $2.36 \text{ Å}^3/\text{Dalton}$ for two molecules (i.e. one ring) per asymmetric unit. The present structure was solved by molecular replacement with the program MOLREP and was refined up to 1.65 Å resolution, which represents an important improvement in comparison to the 2.5 Å resolution obtained for the structure published previously (Kong *et al.*, 1992). The atomic coordinates of the structure solved by the Inventors are given in Figure 1 in pdb format. The superposition of the present structure onto the previous one yields an overall rmsd of 1.22 Å for the C α chain, which indicates that both structures are very similar, although numerous side chains and several mobile loops were rebuilt and a better description of the solvent was achieved. A more sensible superposition, systematically downweighting too distant residues (as those in the rebuilt loops), yields a weighted rmsd of 0.78 Å , which is more significant than the former value.

15 A density related to the presence of the peptide could be located after several rounds of refinement in a "simulated annealing composite omit map" (Brunger *et al.*, 1998). The seven C-terminal residues of the P16 peptide, R₁₀Q₁₁L₁₂V₁₃L₁₄G₁₅L₁₆, encompassing the

β binding sequence were built into the density map (**Figure 2**). This map extended slightly toward the N-terminus of the peptide but rapidly faded, so that the Q₁₁ residue was still easily seen while the R₁₀ was built in a poor density region. The rest of the peptide, probably disordered, was not visible. The seven C-terminal amino acids of the P16 peptide bind onto the β surface within two distinct but adjacent domains: one deep crevice, located between sub-domains 2 and 3 (area 1), and a second area which extends over the third β subdomain, close to the C-terminal extremity of the β chain (area 2) (**Figure 2**).

In the first area (area 1) of the peptide P16 binding site, two β strands of the clamp (β^4 of domain 2 and β^8 of domain 3) align. Some of their residues (L177 and V360, respectively), along with residues of the subdomain connecting loop (P242 and V247), form a hydrophobic pocket at the surface of the β monomer. The P16 residues L16 and L14 bind in this crevice. The hydrophobic nature of the interactions is revealed by the removal, upon peptide binding, of water molecules nested inside the free pocket. However, L14 and L16 are also involved in interactions with other adjacent residues like L155, T172, H175, R176, S346 and M362 (**Table 2**). The residue G15 has no interaction with any residues of the pocket and serves as a connector between L14 and L16. Consequently, the L16 residue which, according to the pentapeptidic consensus motif (Q₁L₂(SD)₃L₄F₅) (Dalrymple *et al.*, 2001), was not considered to belong to the β -binding sequence, actually fully participates to the interaction.

In the second binding area (area 2), the four other P16 residues, V13, L12, Q11 and R10 establish mostly hydrophobic interactions with residues H175, N320, Y323, V344, M362, P363 and M364 of the β monomer (**Table 2**). Among the four P16 residues located within this region, the Q residue is highly conserved within the binding motifs of the various β ligands, to the same extent as residues that bind into the hydrophobic crevice (L14 and L16) (Dalrymple *et al.*, 2001). Particularly, it forms interactions, directly or mediated by two water molecules with β residues M362 and E320. These contacts might prime the binding of the peptide with the β surface and facilitate the formation of interactions of the C-terminal residues within the hydrophobic pocket of area 1. Thus the peptide would be anchored on the β surface by two points located on each extremity of the binding sequence.

β residues	Interacting P16 residues
M364	R10,Q11,L12
P363	Q11, L12
M362	Q11,L12,V13,L14
V361	L14
V344	L12
Y323	Q11
N320	Q11
V360	L14
S346	L14
V247	L14,L16
P242	L16
L177	L14,L16
R176	L14
H175	Q11,L12,V13,L14
T172	L14,L16
L155	L16

Interactions between the β residues and the peptide P16 residues. All considered distances between β and peptide P16 residues are between 3 and 3.8 Å, except those (P16 residues in bold) between L155:L16, T172:L14, L177:L16 and V361:L14 which are larger than 4 Å.

Table 2

5. N-terminal sequencing of the protein

The cristal was recovered after data collection, washed several times in the well solution, and dissolved in 10 μ l water. The proteins contained within the crystal were derivatized and sequenced by automated Edman's degradation using a PE Applied Biosystems 492 cLC Protein Sequencer allowing the identification and precise quantitative analysis of the amino acids released at each step of degradation.

EXAMPLE 2

In vitro study of the β clamp- β binding peptide of Pol IV interaction by competition assays

In order to ascertain the biological relevance of the P16 peptide- β clamp interaction observed in the crystallographic structure, an *in vitro* assay based on the activity of Pol IV DNA polymerase was designed. This assay relies on the observation that the *in vitro* activity of Pol IV is greatly enhanced by the presence of the β subunit loaded onto a primer/template DNA substrate (Wagner *et al.*, 2000) (**Figure 3A**, compare lanes 1 and 5 or 9 and 13), while the enzyme alone incorporates nucleotides in a distributive mode (Wagner *et al.*, 1999).

Briefly, P16 peptide and a control peptide (CLIP) were diluted in 20 mM NaHCO₃ at concentrations of 250, 100 and 10 pmol/μl. 5' end radiolabelling, purification and annealing of synthetic primers were performed as previously described (Wagner *et al.*, 1999). The 30/90 nucleotide synthetic construct (Wagner *et al.*, 2000) was obtained by annealing the 30 nucleotide primer (5'GTAAAACGACGGCCAGTGCCAAGCTTAGTC) (SEQ ID NO : 3) with the 90 nucleotide template (5'CCATGATTACGAATTCAGTCATCACCGGCGC CACAGACTAAGCTTGGCACTGGCCGTCGTTTTACAACGTCGTGACTGGGAAAACC CTGG) (SEQ ID NO : 4) to form a double stranded structure with 5' and 3' single stranded DNA overhangs of 25 and 35 nucleotides, respectively.

All replication experiments (10 μl final volume) were carried out in buffer E (40 mM HEPES pH 7.5, 80 mM potassium glutamate, 160 μg/ml BSA, 16 % glycerol, 0.016 % NP40, 8 mM DTT). The 30/90 nucleotide hybrid was first incubated with single strand binding proteins (SSB; Sigma; 90 nM final concentration) in the presence of ATP (200 μM) and MgCl₂ (7.5 mM) at 37°C for 10 min. When specified, the γ complex (1 nM final concentration) (gift from Dr. C. S. McHenry, Denver, USA), and the β clamp (5 nM as dimer final concentration) were added at that stage, and incubation was carried out at 37°C for 10 min. Then, 7 μl of the mixture was added to 1 μl of either 20 mM NaHCO₃ or 1 μl of peptide solution (1, 10 or 25 μM final concentration), incubated 20 min. at room temperature and further 2 hours at 4°C. 1 μl of polymerase was then added (1.5 nM of Pol IV or 6 nM of α subunit (gift from Dr. H. Maki, Nara, Japan) final concentrations), incubated 5 min. at room temperature and finally, the whole reaction was mixed with 1 μl of a dNTPs solution (200 μM each dNTP final concentration) and let to react for 1 min. at room temperature. Reactions were quenched by the addition of 20 μl of 95 % formamide/dyes solution containing 7.5 mM EDTA, heat-denatured and analysed by chromatography on 12 % denaturing polyacrylamide gels. Radiolabelled products were visualised and quantified using a PhosphorImager 445 SI (Molecular Dynamics) and the ImageQuant software.

As shown in **Figure 3A** and **Figure 3B**, increasing amounts of P16 inhibits the β-dependent activity of Pol IV (lane 13 to 16). At the highest P16 concentration tested (25 μM), the β-dependent Pol IV activity is decreased by a factor around 30, as indicated on the graphic. On the other hand, the control peptide (CLIP) has no effect on this activity even at the highest concentration tested (**Figure 3A**, lane 8). Also, neither P16 nor CLIP peptides do affect the intrinsic activity of Pol IV characterised by the distributive incorporation of one to up to 12 nucleotides (**Figure 3A**, lanes 1-4, 9-12, **Figure 3B**). Thus P16 specifically inhibits

the β -Pol IV DNA polymerase interaction in solution, which demonstrate that the site we identified actually corresponds to the Pol IV DNA polymerase binding site on β .

The polymerase activity of the α subunit of the replicative DNA Polymerase III of *E. coli* is greatly enhanced by its interaction with the β clamp (Marians *et al.*, 1998) (**Figure 3C**, compare lanes 1 and 5 or 9 and 13), and the putative β binding peptide of the α subunit has been identified through bioinformatics analysis (Dalrymple *et al.*, 2001) and is a variant of the pentapeptide consensus motif. In order to determine if the replicative DNA polymerase interact with the β monomer within the same site than Pol IV, the ability of P16 peptide to inhibit the β -dependent activity of the α subunit was tested. The dose dependent inhibition of the α subunit β -dependent activity (**Figure 3C**, lane 13 to 16, **Figure 3D**) strongly suggest that this is the case. To achieve a high level of inhibition, the concentration of P16 peptide should exceed the polymerase concentration by a factor of 4 to $16 \cdot 10^3$. The need for such a high excess of peptide may reflect a higher affinity of the whole protein for the DNA- β substrate, mediated by other polymerase- β and/or polymerase-DNA interactions, but also a high entropic factor of the free peptide as opposed to the same fragment folded in the whole protein. Therefore, the lower peptide affinity would result from a lower kinetic constant k_{on} , and not from an increased k_{off} . Overall, this biochemical analysis indicates that (i) the P16- β structure we solved is of biological significance as indicated by the competitive inhibition of the β dependent activity of Pol IV DNA polymerase by peptide P16 and (ii) that peptide P16 also competes with and inhibits the β dependent activity of the α subunit of the DNA Polymerase III of *E. coli* which suggests that (iii) if not identical, the Pol IV and α subunit interaction sites on β subunit overlap.

EXAMPLE 3

25 *In vivo* study of the inhibition of bacterial growth by the β binding peptide of Pol IV

Plasmids bearing either the wild type Pol IV (pWp4) or the Pol IV mutant deleted for the 5 last C-terminal residues (pD5p4) coding sequences under the IPTG inducible *lac* promoter were transformed into recipient *E. coli* cells (BL21(DE3, pLys)). These transformed cells were then allowed to grow in LB medium at 37°C with aeration and without or with (**Figure 4**) addition of the protein expression inducer IPTG (0.1 mM). Growth rates were monitored by measuring the optical density of the cultures (OD 600 nm) at different time points.

The growth rates of both cultures without artificial protein expression were identical whether the cells contain the wild type Pol IV expression plasmid (pWp4) or the Pol IVD5 mutant (pD5p4). On the other hand, when protein expression was induced by the adjunction of low IPTG concentration in the culture medium (Figure 4), a clear growth inhibition was observed for the culture expressing the wild type Pol IV protein compared to the one expressing the mutant protein. As the mutant protein (expressed from pD5p4) lacks essential amino acids for the interaction with the β -clamp, the observed cytotoxicity may be rationalised by the fact that the wild type Pol IV protein interacts with the β clamp and, because of its relative high concentration, interfere and/or compete with the binding of the replicative DNA polymerase, thereby inhibiting chromosome replication and culture growth.

In other words, these preliminary results indicate that site-specific β binding molecules (such as the Pol IV β binding motif) may serve as antimicrobial agents.

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CLAIMS

1. A protein crystal comprising the processivity clamp factor of DNA polymerase and a peptide of about 3 to about 30 amino acids, in particular of about 16 amino acids, said peptide comprising all or part of the processivity clamp factor binding sequence of a processivity clamp factor interacting protein, such as prokaryotic Pol I, Pol II, Pol III, Pol IV, Pol V, MutS, ligase I, α subunit of DNA polymerase, UmuD or UmuD', or eukaryotic pol ϵ , pol δ , pol η , pol ι , pol κ .

2. A protein crystal according to claim 1, wherein the processivity clamp factor of DNA polymerase is the β subunit of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, and the peptide has the following sequence:

VTLLDPQMERQLVLGL (SEQ ID NO: 1)

3. A protein crystal according to claim 1 or 2, comprising the β subunit of DNA polymerase III of *Escherichia coli* and the peptide of SEQ ID NO: 1, said crystal being triclinic and its cell dimensions being approximately $a = 41.23 \text{ \AA}$, $b = 65.22 \text{ \AA}$, $c = 73.38 \text{ \AA}$, $\alpha = 73.11^\circ$, $\beta = 85.58^\circ$, $\gamma = 85.80^\circ$.

4. A protein crystal according to claim 3, characterized by the atomic coordinates such as obtained by the X-ray diffraction of said crystal, said atomic coordinates being represented in Figure 1.

5. A protein crystal according to claim 3 or 4, characterized by the atomic coordinates representing the peptide and the peptide binding site of the β subunit of DNA polymerase III of *Escherichia coli*, and being as follows:

ATOM	4045	N	LEU B 155	5.874	17.816	22.109	1.00	1.00	B
ATOM	4046	CA	LEU B 155	6.029	16.359	22.087	1.00	1.00	B
ATOM	4047	CB	LEU B 155	5.055	15.686	23.064	1.00	1.00	B
ATOM	4048	CG	LEU B 155	5.260	16.046	24.536	1.00	1.00	B
ATOM	4049	CD1	LEU B 155	4.256	15.237	25.360	1.00	1.00	B
ATOM	4050	CD2	LEU B 155	6.686	15.757	24.980	1.00	1.00	B
ATOM	4051	C	LEU B 155	5.808	15.776	20.682	1.00	1.00	B
ATOM	4052	O	LEU B 155	6.177	14.613	20.431	1.00	1.00	B
ATOM	4177	N	THR B 172	9.112	11.246	22.902	1.00	1.00	B
ATOM	4178	CA	THR B 172	8.212	10.730	23.917	1.00	1.00	B
ATOM	4179	CB	THR B 172	8.776	11.014	25.344	1.00	1.00	B
ATOM	4180	CG1	THR B 172	7.931	10.400	26.328	1.00	1.00	B
ATOM	4181	CG2	THR B 172	8.870	12.532	25.619	1.00	1.00	B
ATOM	4182	C	THR B 172	6.805	11.269	23.709	1.00	1.00	B
ATOM	4183	O	THR B 172	6.588	12.352	23.145	1.00	1.00	B
ATOM	4192	N	GLY B 174	4.562	10.770	26.397	1.00	1.00	B

	ATOM	4193	CA	GLY	B	174	3.992	10.745	27.737	1.00	1.00	
	ATOM	4194	C	GLY	B	174	3.762	9.337	28.266	1.00	1.00	B
	ATOM	4195	O	GLY	B	174	3.667	9.141	29.489	1.00	1.00	B
5	ATOM	4196	N	HIS	B	175	3.650	8.349	27.375	1.00	1.00	B
	ATOM	4197	CA	HIS	B	175	3.440	6.953	27.796	1.00	1.00	B
	ATOM	4198	CB	HIS	B	175	2.313	6.309	26.977	1.00	1.00	B
	ATOM	4199	CG	HIS	B	175	0.992	6.997	27.119	1.00	1.00	B
	ATOM	4200	CD2	HIS	B	175	0.106	7.435	26.193	1.00	1.00	B
10	ATOM	4201	ND1	HIS	B	175	0.420	7.255	28.345	1.00	1.00	B
	ATOM	4202	CE1	HIS	B	175	-0.763	7.817	28.170	1.00	1.00	B
	ATOM	4203	NE2	HIS	B	175	-0.977	7.938	26.875	1.00	1.00	B
	ATOM	4204	C	HIS	B	175	4.706	6.135	27.641	1.00	1.00	B
	ATOM	4205	O	HIS	B	175	4.990	5.212	28.403	1.00	1.00	B
15	ATOM	4206	N	ARG	B	176	5.481	6.461	26.617	1.00	18.76	B
	ATOM	4207	CA	ARG	B	176	6.711	5.768	26.422	1.00	18.30	B
	ATOM	4208	CB	ARG	B	176	6.575	4.633	25.398	1.00	19.53	B
	ATOM	4209	CG	ARG	B	176	6.329	5.094	23.954	1.00	22.88	B
	ATOM	4210	CD	ARG	B	176	4.876	4.888	23.657	1.00	22.11	B
20	ATOM	4211	NE	ARG	B	176	4.435	5.312	22.314	1.00	22.09	B
	ATOM	4212	CZ	ARG	B	176	4.555	4.591	21.202	1.00	20.17	B
	ATOM	4213	NH1	ARG	B	176	5.159	3.403	21.213	1.00	17.04	B
	ATOM	4214	NH2	ARG	B	176	3.914	4.977	20.120	1.00	20.02	B
	ATOM	4215	C	ARG	B	176	7.684	6.807	25.902	1.00	17.30	B
25	ATOM	4216	O	ARG	B	176	7.255	7.860	25.374	1.00	18.10	B
	ATOM	4217	N	LEU	B	177	8.957	6.504	26.080	1.00	17.97	B
	ATOM	4218	CA	LEU	B	177	10.049	7.360	25.633	1.00	17.85	B
	ATOM	4219	CB	LEU	B	177	10.664	8.095	26.827	1.00	18.29	B
	ATOM	4220	CG	LEU	B	177	11.921	8.955	26.611	1.00	16.28	B
30	ATOM	4221	CD1	LEU	B	177	11.819	10.163	27.559	1.00	19.52	B
	ATOM	4222	CD2	LEU	B	177	13.191	8.172	26.839	1.00	19.12	B
	ATOM	4223	C	LEU	B	177	11.110	6.517	24.964	1.00	18.45	B
	ATOM	4224	O	LEU	B	177	11.291	5.329	25.281	1.00	18.33	B
	ATOM	4710	N	PRO	B	242	11.254	17.279	27.890	1.00	1.00	B
35	ATOM	4711	CD	PRO	B	242	9.987	16.826	27.286	1.00	1.00	B
	ATOM	4712	CA	PRO	B	242	11.660	16.404	28.997	1.00	1.00	B
	ATOM	4713	CB	PRO	B	242	10.688	15.230	28.874	1.00	1.00	B
	ATOM	4714	CG	PRO	B	242	9.448	15.869	28.336	1.00	1.00	B
	ATOM	4715	C	PRO	B	242	13.124	15.947	28.987	1.00	1.00	B
40	ATOM	4716	O	PRO	B	242	13.728	15.748	27.925	1.00	1.00	B
	ATOM	4748	N	ARG	B	246	16.133	11.840	33.560	1.00	1.00	B
	ATOM	4749	CA	ARG	B	246	15.239	11.808	34.707	1.00	1.00	B
	ATOM	4750	CB	ARG	B	246	14.755	13.227	34.984	1.00	1.00	B
	ATOM	4751	CG	ARG	B	246	15.880	14.252	35.113	1.00	1.00	B
45	ATOM	4752	CD	ARG	B	246	16.443	14.295	36.529	1.00	1.00	B
	ATOM	4753	NE	ARG	B	246	15.374	14.318	37.524	1.00	1.00	B
	ATOM	4754	CZ	ARG	B	246	14.316	15.126	37.477	1.00	1.00	B
	ATOM	4755	NH1	ARG	B	246	14.169	15.992	36.481	1.00	1.00	B
	ATOM	4756	NH2	ARG	B	246	13.396	15.067	38.430	1.00	1.00	B
50	ATOM	4757	C	ARG	B	246	14.022	10.889	34.566	1.00	1.00	B
	ATOM	4758	O	ARG	B	246	13.384	10.536	35.560	1.00	1.00	B
	ATOM	4759	N	VAL	B	247	13.695	10.532	33.327	1.00	1.00	B
	ATOM	4760	CA	VAL	B	247	12.553	9.675	33.018	1.00	1.00	B
	ATOM	4761	CB	VAL	B	247	12.061	9.942	31.585	1.00	1.00	B
55	ATOM	4762	CG1	VAL	B	247	10.930	8.991	31.216	1.00	1.00	B
	ATOM	4763	CG2	VAL	B	247	11.624	11.391	31.462	1.00	1.00	B
	ATOM	4764	C	VAL	B	247	12.962	8.218	33.133	1.00	1.00	B
	ATOM	4765	O	VAL	B	247	12.125	7.334	33.308	1.00	1.00	B
60	ATOM	4996	N	PHE	B	278	-7.702	-1.352	24.244	1.00	1.00	B
	ATOM	4997	CA	PHE	B	278	-6.698	-1.155	25.300	1.00	1.00	B
	ATOM	4998	CB	PHE	B	278	-7.318	-1.432	26.663	1.00	1.00	B
	ATOM	4999	CG	PHE	B	278	-8.431	-0.459	27.021	1.00	1.00	B
	ATOM	5000	CD1	PHE	B	278	-8.142	0.882	27.268	1.00	1.00	B
	ATOM	5001	CD2	PHE	B	278	-9.760	-0.869	27.021	1.00	1.00	B
65	ATOM	5002	CE1	PHE	B	278	-9.177	1.816	27.508	1.00	1.00	B
	ATOM	5003	CE2	PHE	B	278	-10.795	0.052	27.258	1.00	1.00	B
	ATOM	5004	CZ	PHE	B	278	-10.496	1.391	27.500	1.00	1.00	B
	ATOM	5005	C	PHE	B	278	-5.403	-1.957	25.131	1.00	1.00	B
	ATOM	5006	O	PHE	B	278	-4.356	-1.582	25.677	1.00	1.00	B
70	ATOM	5332	N	ASN	B	320	0.635	-2.143	27.431	1.00	1.00	B
	ATOM	5333	CA	ASN	B	320	-0.051	-1.983	26.158	1.00	1.00	B
	ATOM	5334	CB	ASN	B	320	-0.055	-0.504	25.796	1.00	1.00	B
	ATOM	5335	CG	ASN	B	320	-0.561	-0.259	24.407	1.00	1.00	B
	ATOM	5336	OD1	ASN	B	320	-0.226	-0.997	23.481	1.00	1.00	B
75	ATOM	5337	ND2	ASN	B	320	-1.362	0.791	24.242	1.00	1.00	B
	ATOM	5338	C	ASN	B	320	0.927	-2.748	25.249	1.00	1.00	B
	ATOM	5339	O	ASN	B	320	2.093	-2.350	25.102	1.00	1.00	B
	ATOM	5353	N	TYR	B	323	2.932	-0.853	22.482	1.00	1.00	B

	ATOM	5354	CA	TYR	B	323	4.110	-0.088	22.908	1.00	1.00	
	ATOM	5355	CB	TYR	B	323	3.878	0.590	24.259	1.00	1.00	B
	ATOM	5356	CG	TYR	B	323	2.813	1.668	24.294	1.00	1.00	B
5	ATOM	5357	CD1	TYR	B	323	2.397	2.314	23.127	1.00	1.00	B
	ATOM	5358	CE1	TYR	B	323	1.458	3.374	23.170	1.00	1.00	B
	ATOM	5359	CD2	TYR	B	323	2.284	2.093	25.509	1.00	1.00	B
	ATOM	5360	CE2	TYR	B	323	1.354	3.166	25.567	1.00	1.00	B
	ATOM	5361	CZ	TYR	B	323	0.957	3.790	24.399	1.00	1.00	B
10	ATOM	5362	OH	TYR	B	323	0.112	4.886	24.453	1.00	1.00	B
	ATOM	5363	C	TYR	B	323	5.327	-1.018	23.041	1.00	1.00	B
	ATOM	5364	O	TYR	B	323	6.468	-0.646	22.726	1.00	1.00	B
	ATOM	5519	N	VAL	B	344	3.837	-1.100	39.291	1.00	1.00	B
	ATOM	5520	CA	VAL	B	344	3.324	0.227	39.030	1.00	1.00	B
15	ATOM	5521	CB	VAL	B	344	2.676	0.818	40.318	1.00	1.00	B
	ATOM	5522	CG1	VAL	B	344	1.474	-0.026	40.725	1.00	1.00	B
	ATOM	5523	CG2	VAL	B	344	3.687	0.847	41.456	1.00	1.00	B
	ATOM	5524	C	VAL	B	344	4.405	1.163	38.512	1.00	1.00	B
	ATOM	5525	O	VAL	B	344	4.199	2.365	38.405	1.00	1.00	B
20	ATOM	5532	N	SER	B	346	7.618	2.153	35.615	1.00	21.53	B
	ATOM	5533	CA	SER	B	346	8.060	2.002	34.239	1.00	21.50	B
	ATOM	5534	CB	SER	B	346	8.655	3.320	33.722	1.00	21.47	B
	ATOM	5535	OG	SER	B	346	9.793	3.703	34.474	1.00	26.08	B
	ATOM	5536	C	SER	B	346	9.107	0.914	34.106	1.00	20.70	B
25	ATOM	5537	O	SER	B	346	9.755	0.521	35.078	1.00	21.55	B
	ATOM	5632	N	VAL	B	360	11.730	3.546	27.545	1.00	1.00	B
	ATOM	5633	CA	VAL	B	360	11.023	3.501	28.812	1.00	1.00	B
	ATOM	5634	CB	VAL	B	360	11.276	4.794	29.641	1.00	1.00	B
	ATOM	5635	CG1	VAL	B	360	10.448	4.742	30.934	1.00	1.00	B
30	ATOM	5636	CG2	VAL	B	360	12.753	4.923	29.937	1.00	1.00	B
	ATOM	5637	C	VAL	B	360	9.562	3.381	28.501	1.00	1.00	B
	ATOM	5638	O	VAL	B	360	9.008	4.188	27.753	1.00	1.00	B
	ATOM	5639	N	VAL	B	361	8.905	2.372	29.069	1.00	19.72	B
35	ATOM	5640	CA	VAL	B	361	7.488	2.188	28.831	1.00	18.92	B
	ATOM	5641	CB	VAL	B	361	7.216	0.872	28.069	1.00	18.99	B
	ATOM	5642	CG1	VAL	B	361	5.743	0.769	27.716	1.00	18.31	B
	ATOM	5643	CG2	VAL	B	361	8.065	0.839	26.786	1.00	17.76	B
	ATOM	5644	C	VAL	B	361	6.793	2.100	30.167	1.00	19.47	B
40	ATOM	5645	O	VAL	B	361	7.232	1.362	31.038	1.00	16.90	B
	ATOM	5646	N	MET	B	362	5.737	2.885	30.318	1.00	1.00	B
	ATOM	5647	CA	MET	B	362	4.962	2.882	31.540	1.00	1.00	B
	ATOM	5648	CB	MET	B	362	4.226	4.206	31.682	1.00	1.00	B
	ATOM	5649	CG	MET	B	362	3.918	4.589	33.122	1.00	1.00	B
	ATOM	5650	SD	MET	B	362	5.405	4.806	34.163	1.00	1.00	B
45	ATOM	5651	CE	MET	B	362	4.575	4.880	35.731	1.00	1.00	B
	ATOM	5652	C	MET	B	362	3.949	1.731	31.471	1.00	1.00	B
	ATOM	5653	O	MET	B	362	3.385	1.438	30.410	1.00	1.00	B
	ATOM	5654	N	PRO	B	363	3.698	1.069	32.599	1.00	1.00	B
	ATOM	5655	CD	PRO	B	363	4.521	1.025	33.818	1.00	1.00	B
50	ATOM	5656	CA	PRO	B	363	2.729	-0.038	32.579	1.00	1.00	B
	ATOM	5657	CB	PRO	B	363	3.155	-0.883	33.776	1.00	1.00	B
	ATOM	5658	CG	PRO	B	363	3.665	0.160	34.754	1.00	1.00	B
	ATOM	5659	C	PRO	B	363	1.272	0.395	32.672	1.00	1.00	B
	ATOM	5660	O	PRO	B	363	0.959	1.574	32.811	1.00	1.00	B
55	ATOM	5661	N	MET	B	364	0.368	-0.568	32.537	1.00	1.00	B
	ATOM	5662	CA	MET	B	364	-1.037	-0.272	32.674	1.00	1.00	B
	ATOM	5663	CB	MET	B	364	-1.780	-0.391	31.332	1.00	1.00	B
	ATOM	5664	CG	MET	B	364	-1.636	-1.670	30.568	1.00	1.00	B
	ATOM	5665	SD	MET	B	364	-2.386	-1.510	28.872	1.00	1.00	B
60	ATOM	5666	CE	MET	B	364	-4.155	-1.253	29.308	1.00	1.00	B
	ATOM	5667	C	MET	B	364	-1.602	-1.218	33.725	1.00	1.00	B
	ATOM	5668	O	MET	B	364	-0.999	-2.251	34.035	1.00	1.00	B
	ATOM	5669	N	ARG	B	365	-2.732	-0.836	34.307	1.00	1.00	B
65	ATOM	5670	CA	ARG	B	365	-3.383	-1.655	35.324	1.00	1.00	B
	ATOM	5671	CB	ARG	B	365	-4.029	-0.756	36.394	1.00	1.00	B
	ATOM	5672	CG	ARG	B	365	-4.785	-1.490	37.505	1.00	1.00	B
	ATOM	5673	CD	ARG	B	365	-3.859	-2.316	38.398	1.00	1.00	B
	ATOM	5674	NE	ARG	B	365	-4.571	-2.956	39.505	1.00	1.00	B
	ATOM	5675	CZ	ARG	B	365	-3.984	-3.707	40.434	1.00	1.00	B
70	ATOM	5676	NH1	ARG	B	365	-2.678	-3.913	40.385	1.00	1.00	B
	ATOM	5677	NH2	ARG	B	365	-4.698	-4.247	41.418	1.00	1.00	B
	ATOM	5678	C	ARG	B	365	-4.459	-2.492	34.648	1.00	1.00	B
	ATOM	5679	O	ARG	B	365	-5.449	-1.961	34.150	1.00	1.00	B
75	ATOM	5680	N	LEU	B	366	-4.267	-3.801	34.609	1.00	41.59	B
	ATOM	5681	CA	LEU	B	366	-5.272	-4.665	33.996	1.00	44.25	B
	ATOM	5682	CB	LEU	B	366	-4.615	-5.908	33.366	1.00	45.24	B
	ATOM	5683	CG	LEU	B	366	-3.640	-5.701	32.202	1.00	45.46	B
	ATOM	5684	CD1	LEU	B	366	-4.331	-5.029	31.031	1.00	47.09	B

	ATOM	5685	CD2	LEU	B	366	-2.489	-4.856	32.678	1.00	46.71	
	ATOM	5686	C	LEU	B	366	-6.263	-5.080	35.092	1.00	45.55	B
	ATOM	5687	O	LEU	B	366	-6.424	-6.296	35.333	1.00	46.32	B
5	ATOM	5688	OXT	LEU	B	366	-6.868	-4.169	35.704	1.00	46.33	B
	ATOM	5689	CB	ARG	C	10	-5.663	0.205	32.737	0.76	1.00	C
	ATOM	5690	CG	ARG	C	10	-7.073	-0.397	32.771	0.76	1.00	C
	ATOM	5691	CD	ARG	C	10	-7.748	-0.383	31.408	0.76	1.00	C
	ATOM	5692	NE	ARG	C	10	-8.728	-1.462	31.268	0.76	1.00	C
10	ATOM	5693	CZ	ARG	C	10	-9.992	-1.301	30.875	0.76	1.00	C
	ATOM	5694	NH1	ARG	C	10	-10.464	-0.093	30.582	0.76	1.00	C
	ATOM	5695	NH2	ARG	C	10	-10.779	-2.365	30.749	0.76	1.00	C
	ATOM	5696	C	ARG	C	10	-4.106	2.152	32.497	0.76	1.00	C
	ATOM	5697	O	ARG	C	10	-3.278	1.863	33.369	0.76	1.00	C
15	ATOM	5698	N	ARG	C	10	-6.417	2.186	31.464	0.76	1.00	C
	ATOM	5699	CA	ARG	C	10	-5.587	1.727	32.625	0.76	1.00	C
	ATOM	5700	N	GLN	C	11	-3.805	2.853	31.408	0.76	1.00	C
	ATOM	5701	CA	GLN	C	11	-2.458	3.321	31.094	0.76	1.00	C
	ATOM	5702	CB	GLN	C	11	-2.423	3.866	29.662	0.76	1.00	C
20	ATOM	5703	CG	GLN	C	11	-1.047	4.361	29.231	0.76	1.00	C
	ATOM	5704	CD	GLN	C	11	-0.039	3.245	29.174	0.76	1.00	C
	ATOM	5705	OE1	GLN	C	11	-0.263	2.232	28.494	0.76	1.00	C
	ATOM	5706	NE2	GLN	C	11	1.082	3.415	29.876	0.76	1.00	C
	ATOM	5707	C	GLN	C	11	-1.895	4.396	32.038	0.76	1.00	C
25	ATOM	5708	O	GLN	C	11	-2.494	5.467	32.217	0.76	1.00	C
	ATOM	5709	N	LEU	C	12	-0.732	4.111	32.618	0.76	1.00	C
	ATOM	5710	CA	LEU	C	12	-0.065	5.046	33.519	0.76	1.00	C
	ATOM	5711	CB	LEU	C	12	0.754	4.277	34.561	0.76	1.00	C
	ATOM	5712	CG	LEU	C	12	-0.036	3.305	35.450	0.76	1.00	C
30	ATOM	5713	CD1	LEU	C	12	0.907	2.681	36.468	0.76	1.00	C
	ATOM	5714	CD2	LEU	C	12	-1.184	4.040	36.153	0.76	1.00	C
	ATOM	5715	C	LEU	C	12	0.845	5.948	32.680	0.76	1.00	C
	ATOM	5716	O	LEU	C	12	1.111	5.653	31.510	0.76	1.00	C
	ATOM	5717	N	VAL	C	13	1.317	7.044	33.273	0.76	1.00	C
35	ATOM	5718	CA	VAL	C	13	2.166	7.987	32.543	0.76	1.00	C
	ATOM	5719	CB	VAL	C	13	1.473	9.371	32.386	0.76	1.00	C
	ATOM	5720	CG1	VAL	C	13	0.217	9.239	31.523	0.76	1.00	C
	ATOM	5721	CG2	VAL	C	13	1.113	9.929	33.750	0.76	1.00	C
	ATOM	5722	C	VAL	C	13	3.542	8.211	33.174	0.76	1.00	C
40	ATOM	5723	O	VAL	C	13	3.740	8.050	34.381	0.76	1.00	C
	ATOM	5724	N	LEU	C	14	4.498	8.596	32.339	0.76	1.00	C
	ATOM	5725	CA	LEU	C	14	5.860	8.846	32.803	0.76	1.00	C
	ATOM	5726	CB	LEU	C	14	6.836	8.819	31.619	0.76	1.00	C
	ATOM	5727	CG	LEU	C	14	6.972	7.481	30.889	0.76	1.00	C
45	ATOM	5728	CD1	LEU	C	14	7.666	7.705	29.557	0.76	1.00	C
	ATOM	5729	CD2	LEU	C	14	7.744	6.495	31.769	0.76	1.00	C
	ATOM	5730	C	LEU	C	14	6.010	10.186	33.517	0.76	1.00	C
	ATOM	5731	O	LEU	C	14	5.238	11.126	33.284	0.76	1.00	C
	ATOM	5732	N	GLY	C	15	7.000	10.263	34.396	0.76	1.00	C
50	ATOM	5733	CA	GLY	C	15	7.264	11.510	35.090	0.76	1.00	C
	ATOM	5734	C	GLY	C	15	8.263	12.275	34.234	0.76	1.00	C
	ATOM	5735	O	GLY	C	15	9.472	12.210	34.462	0.76	1.00	C
	ATOM	5736	N	LEU	C	16	7.750	12.995	33.241	0.76	1.00	C
	ATOM	5737	CA	LEU	C	16	8.576	13.756	32.306	0.76	1.00	C
55	ATOM	5738	CB	LEU	C	16	7.732	14.157	31.094	0.76	1.00	C
	ATOM	5739	CG	LEU	C	16	7.258	12.955	30.269	0.76	1.00	C
	ATOM	5740	CD1	LEU	C	16	6.303	13.411	29.171	0.76	1.00	C
	ATOM	5741	CD2	LEU	C	16	8.467	12.233	29.690	0.76	1.00	C
	ATOM	5742	C	LEU	C	16	9.263	14.982	32.898	0.76	1.00	C
60	ATOM	5743	O	LEU	C	16	10.182	15.515	32.231	0.76	1.00	C
	ATOM	5744	OXT	LEU	C	16	8.870	15.398	34.009	0.76	1.00	C
	END											

wherein atoms 4045 to 5688 represent the peptide binding site and atoms 5689 to 5748 represent the peptide.

65 6. A method to purify the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, comprising the following steps:

- elution of a solution containing the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, through a cation exchange column, in particular a SP sepharose column;

- elution of a solution containing the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, in particular as obtained by the preceding step, through an anion exchange column, in particular a Mono Q column;

- elution of a solution containing the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, in particular as obtained by the preceding step, through a cation exchange column, in particular a Mono S column.

7. A method to obtain a protein crystal as defined in claims 1 to 5, comprising the following steps:

- mixing a solution of processivity clamp factor of DNA polymerase, with a solution of a peptide of about 3 to about 30 amino acids, in particular of about 16 amino acids, said peptide comprising all or part of the processivity clamp factor binding sequence of a processivity clamp factor interacting protein, such as prokaryotic Pol I, Pol II, Pol III, Pol IV, Pol V, MutS, ligase I, α subunit of DNA polymerase, UmuD or UmuD', or eukaryotic pol ϵ , pol δ , pol η , pol ι , pol κ , and with a solution of MES pH 6.0 0.2 M, CaCl_2 0.2 M, PEG 400 60%, to obtain a crystallisation drop,

- letting the crystallisation drop concentrate against a solution of MES pH 6.0 0.1 M, CaCl_2 0.1 M, PEG 400 30%, by vapour diffusion, to obtain a protein crystal.

8. A method according to claim 7, wherein the processivity clamp factor of DNA polymerase is the β subunit of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*, in particular as purified according to claim 6, and the peptide has the following sequence:

VTLLDPQMERQLVLGL (SEQ ID NO: 1).

9. The use of the atomic coordinates as defined in claims 4 and 5, for the screening, the design or the modification of ligands of the processivity clamp factor of DNA polymerase, in particular of the β subunit of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*.

10. The use according to claim 9, for the screening, the design or the modification of ligands liable to be used for the preparation of pharmaceutical compositions useful for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or proliferative disorders, such as cancers.

11. A method to screen ligands of the processivity clamp factor of DNA polymerase, said method comprising the step of assessing the interaction of tridimensional models of the ligands to screen with the structure of the β subunit of DNA polymerase as defined by the atomic coordinates according to claim 4, and in particular with the structure of the peptide binding site as defined by the atomic coordinates according to claim 5, and more particularly with at least nine of the following amino acids: Leu 155, Thr 172, Gly 174, His 175, Arg 176, Leu 177, Pro 242, Arg 246, Val 247, Phe 278, Asn 320, Tyr 323, Val 344, Ser 346, Val 360, Val 361, Met 362, Pro 363, Met 364, Arg 365, Leu 366.

12. A method according to claim 11, to screen ligands liable to be used for the preparation of pharmaceutical compositions useful for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or proliferative disorders, such as cancers.

13. A method to design or to modify compounds liable to bind to the processivity clamp factor of DNA polymerase, said method comprising the step of designing or modifying a compound, so that the tridimensional model of said compound is liable to interact with the structure of the β subunit of DNA polymerase as defined by the atomic coordinates according to claim 4, and in particular with the structure of the peptide binding site as defined by the atomic coordinates according to claim 5, and more particularly with at least nine of the following amino acids: Leu 155, Thr 172, Gly 174,

His 175, Arg 176, Leu 177, Pro 242, Arg 246, Val 247, Phe 278, Asn 320, Tyr 323, Val 344, Ser 346, Val 360, Val 361, Met 362, Pro 363, Met 364, Arg 365, Leu 366.

5 14. A method according to claim 13, to design or to modify ligands liable to be used for the preparation of pharmaceutical compositions useful for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or proliferative disorders, such as cancers.

10 15. A peptide of the following sequence:

VTLLDPQMERQLVLGL (SEQ ID NO: 1).

16. A pharmaceutical composition comprising as active substance the peptide of claim 15 in association with a pharmaceutically acceptable carrier.

15 17. The use of the peptide of claim 15 as an anti-bacterial compound.

18. The use of the peptide of claim 15 for the manufacture of a medicament for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or of proliferative disorders, such as cancers.

20 19. A method to test in vitro the inhibitory effect of compounds on the processivity clamp factor-dependant activity of DNA polymerase, in particular of Pol IV DNA polymerase of *Escherichia coli*, or of the α subunit of Pol III DNA polymerase of *Escherichia coli*, comprising the following steps:

25 - adding to assay solutions comprising a labelled nucleotidic primer, a template DNA, and DNA polymerase, in particular Pol IV DNA polymerase of *Escherichia coli*, or the α subunit of Pol III DNA polymerase of *Escherichia coli*, a compound to test at a given concentration for each assay solution, in the presence or the absence of the processivity clamp factor of DNA polymerase, in particular the β subunit of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*.

30 - electrophoretically migrating the abovementioned assay solutions,

- comparing the migration pattern of each assay solutions in the presence or the absence of the processivity clamp factor of DNA polymerase, in particular the β subunit

of DNA polymerase, in particular the β subunit of DNA polymerase III of *Escherichia coli*.

5 20. The use of a method according to claim 19, for the screening of compounds liable to be used for the preparation of pharmaceutical compositions useful for the treatment of bacterial diseases or diseases originating from DNA synthesis processes, such as fragile X syndrome, or proliferative disorders, such as cancers.

ABSTRACT

5 The present invention relates to a protein crystal comprising the processivity clamp factor of DNA polymerase and a peptide of about 3 to about 30 amino acids, in particular of about 16 amino acids, said peptide comprising all or part of the processivity clamp factor binding sequence of a processivity clamp factor interacting protein, such as prokaryotic Pol I, Pol II, Pol III, Pol IV, Pol V, MutS, ligase I, α subunit of DNA polymerase, UmuD or UmuD', or eukaryotic pol ϵ , pol δ , pol η , pol ι , pol κ .

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(no drawing)

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REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 500.0 - 1.65 Å
REMARK starting r= 0.2072 free r= 0.2361
REMARK final r= 0.2072 free r= 0.2361
REMARK B rmsd for bonded mainchain atoms= 1.427 target= 1.5
REMARK B rmsd for bonded sidechain atoms= 2.420 target= 2.0
REMARK B rmsd for angle mainchain atoms= 2.189 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.637 target= 2.5
REMARK rweight= 0.1000 (with wa= 0.987736)
REMARK target= mlf steps= 30
REMARK sg= P1 a= 41.23 b= 65.22 c= 73.38 alpha= 73.11 beta= 85.58 gamma= 85.8
REMARK parameter file 1 : CNS TOPPAR:protein_rep.param
REMARK parameter file 2 : CNS TOPPAR:water_rep.param
REMARK molecular structure file: amy.mtf
REMARK input coordinates: amy.pdb
REMARK reflection file= amy.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.65
REMARK initial B-factor correction applied to fobs :
REMARK B11= -3.662 B22= 2.485 B33= 1.177
REMARK B12= 2.042 B13= 2.748 B23= -0.502
REMARK B-factor correction applied to coordinate array B: 0.012
REMARK bulk solvent: density level= 0.36444 e/Å³, B-factor= 46.0136 Å²
REMARK reflections with |Fobs|/sigma F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected
REMARK theoretical total number of refl. in resol. range: 87646 { 100.0 % }
REMARK number of unobserved reflections (no entry or |F|=0): 2854 { 3.3 % }
REMARK number of reflections rejected: 0 { 0.0 % }
REMARK total number of reflections used: 84792 { 96.7 % }
REMARK number of reflections in working set: 80566 { 91.9 % }
REMARK number of reflections in test set: 4226 { 4.8 % }
CRYST1 41.230 65.220 73.380 73.11 85.58 85.80 P 1
REMARK FILENAME="/work/olieric/db/db2-5 P1/cns/bindividual.pdb"
REMARK DATE:31-Mar-03 11:57:01
REMARK VERSION:1.1 created by user: olieric
ATOM 1 CB MET A 1 -14.276 -31.220 16.788 1.00 17.29 A
ATOM 2 CG MET A 1 -13.562 -30.976 15.453 1.00 19.06 A
ATOM 3 SD MET A 1 -13.791 -29.325 14.750 1.00 20.01 A
ATOM 4 CE MET A 1 -12.595 -28.385 15.663 1.00 20.04 A
ATOM 5 C MET A 1 -12.346 -32.264 17.931 1.00 17.38 A
ATOM 6 O MET A 1 -12.094 -31.451 18.823 1.00 18.05 A
ATOM 7 N MET A 1 -14.641 -32.810 18.672 1.00 17.69 A
ATOM 8 CA MET A 1 -13.789 -32.489 17.479 1.00 17.26 A
ATOM 9 N LYS A 2 -11.404 -32.959 17.305 1.00 16.63 A
ATOM 10 CA LYS A 2 -9.991 -32.827 17.687 1.00 17.10 A
ATOM 11 CB LYS A 2 -9.686 -33.813 18.819 1.00 20.78 A
ATOM 12 CG LYS A 2 -8.255 -33.915 19.217 1.00 24.62 A
ATOM 13 CD LYS A 2 -8.095 -34.972 20.295 1.00 28.83 A
ATOM 14 CE LYS A 2 -6.710 -34.905 20.918 1.00 31.65 A
ATOM 15 NZ LYS A 2 -6.617 -35.825 22.100 1.00 33.43 A
ATOM 16 C LYS A 2 -9.119 -33.168 16.483 1.00 17.18 A
ATOM 17 O LYS A 2 -9.455 -34.064 15.706 1.00 14.51 A
ATOM 18 N PHE A 3 -8.034 -32.423 16.284 1.00 14.64 A
ATOM 19 CA PHE A 3 -7.135 -32.762 15.187 1.00 14.50 A
ATOM 20 CB PHE A 3 -7.652 -32.265 13.810 1.00 16.07 A
ATOM 21 CG PHE A 3 -7.818 -30.761 13.686 1.00 15.16 A
ATOM 22 CD1 PHE A 3 -9.067 -30.157 13.880 1.00 15.68 A
ATOM 23 CD2 PHE A 3 -6.737 -29.955 13.299 1.00 12.43 A
ATOM 24 CE1 PHE A 3 -9.233 -28.776 13.690 1.00 15.69 A
ATOM 25 CE2 PHE A 3 -6.888 -28.598 13.109 1.00 15.35 A
ATOM 26 CZ PHE A 3 -8.163 -27.996 13.313 1.00 14.58 A
ATOM 27 C PHE A 3 -5.783 -32.146 15.480 1.00 15.40 A
ATOM 28 O PHE A 3 -5.685 -31.234 16.283 1.00 14.89 A
ATOM 29 N THR A 4 -4.732 -32.697 14.884 1.00 13.77 A
ATOM 30 CA THR A 4 -3.407 -32.124 15.046 1.00 15.62 A
ATOM 31 CB THR A 4 -2.486 -32.956 15.948 1.00 17.56 A
ATOM 32 OG1 THR A 4 -3.030 -32.988 17.274 1.00 18.68 A
ATOM 33 CG2 THR A 4 -1.084 -32.288 16.013 1.00 18.01 A
ATOM 34 C THR A 4 -2.846 -32.111 13.645 1.00 15.42 A
ATOM 35 O THR A 4 -2.880 -33.120 12.942 1.00 17.97 A
ATOM 36 N VAL A 5 -2.317 -30.970 13.238 1.00 16.55 A
ATOM 37 CA VAL A 5 -1.804 -30.886 11.883 1.00 16.64 A
ATOM 38 CB VAL A 5 -2.948 -30.508 10.930 1.00 18.41 A
ATOM 39 CG1 VAL A 5 -3.416 -29.040 11.181 1.00 18.38 A
ATOM 40 CG2 VAL A 5 -2.514 -30.773 9.468 1.00 19.99 A
ATOM 41 C VAL A 5 -0.679 -29.886 11.773 1.00 17.93 A
ATOM 42 O VAL A 5 -0.559 -28.960 12.592 1.00 16.18 A
ATOM 43 N GLU A 6 0.166 -30.070 10.765 1.00 16.71 A
ATOM 44 CA GLU A 6 1.253 -29.120 10.579 1.00 18.01 A
ATOM 45 CB GLU A 6 2.218 -29.605 9.499 1.00 19.85 A
ATOM 46 CG GLU A 6 3.012 -30.850 9.875 1.00 24.39 A
ATOM 47 CD GLU A 6 3.999 -31.273 8.780 1.00 30.54 A
ATOM 48 OE1 GLU A 6 4.475 -30.396 8.006 1.00 30.19 A
ATOM 49 OE2 GLU A 6 4.317 -32.484 8.709 1.00 31.65 A
ATOM 50 C GLU A 6 0.734 -27.751 10.164 1.00 17.50 A
ATOM 51 O GLU A 6 -0.166 -27.642 9.334 1.00 17.39 A
ATOM 52 N ARG A 7 1.337 -26.703 10.717 1.00 15.98 A
ATOM 53 CA ARG A 7 0.975 -25.341 10.359 1.00 16.73 A
ATOM 54 CB ARG A 7 1.939 -24.375 11.051 1.00 16.92 A
ATOM 55 CG ARG A 7 1.902 -22.950 10.542 1.00 15.16 A
ATOM 56 CD ARG A 7 3.010 -22.130 11.223 1.00 15.81 A
ATOM 57 NE ARG A 7 3.117 -20.745 10.778 1.00 16.48 A
ATOM 58 CZ ARG A 7 3.906 -20.342 9.787 1.00 19.48 A
ATOM 59 NH1 ARG A 7 4.650 -21.243 9.135 1.00 19.10 A
ATOM 60 NH2 ARG A 7 3.953 -19.063 9.445 1.00 19.15 A
ATOM 61 C ARG A 7 1.077 -25.168 8.842 1.00 19.33 A
ATOM 62 O ARG A 7 0.232 -24.536 8.201 1.00 20.23 A
ATOM 63 N GLU A 8 2.116 -25.777 8.284 1.00 20.57 A
ATOM 64 CA GLU A 8 2.392 -25.680 6.869 1.00 23.30 A
ATOM 65 CB GLU A 8 3.669 -26.474 6.585 1.00 25.23 A

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Figure 1 (1)

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Figure 1 (continued 2)

ATOM	166	CB	LEU	A	21	-13.417	-11.843	6.292	1.00	68.85
ATOM	167	CG	LEU	A	21	-13.658	-11.701	7.797	1.00	69.20
ATOM	168	CD1	LEU	A	21	-15.091	-11.257	8.058	1.00	69.44
ATOM	169	CD2	LEU	A	21	-13.383	-13.037	8.473	1.00	69.17
ATOM	170	C	O	N	21	-12.744	-9.468	5.837	1.00	69.92
ATOM	171	C	O	N	21	-11.823	-9.033	5.133	1.00	70.14
ATOM	172	CA	GLY	A	22	-13.029	-8.981	7.043	1.00	70.90
ATOM	173	CA	GLY	A	22	-12.270	-7.883	7.608	1.00	72.13
ATOM	174	C	O	N	22	-13.141	-6.650	7.685	1.00	73.06
ATOM	175	C	O	N	22	-13.445	-6.156	8.773	1.00	73.37
ATOM	176	CA	GLY	A	23	-13.556	-6.165	6.518	1.00	73.72
ATOM	177	CA	GLY	A	23	-14.395	-4.982	6.447	1.00	74.24
ATOM	178	C	O	N	23	-15.796	-5.167	7.006	1.00	74.63
ATOM	179	C	O	N	23	-16.645	-5.826	6.394	1.00	74.77
ATOM	180	N	ARG	A	24	-16.028	-4.573	8.176	1.00	74.56
ATOM	181	CA	ARG	A	24	-17.315	-4.624	8.865	1.00	74.14
ATOM	182	CB	ARG	A	24	-18.178	-3.428	8.440	1.00	75.43
ATOM	183	CG	ARG	A	24	-19.494	-3.302	9.198	1.00	77.04
ATOM	184	CD	ARG	A	24	-20.297	-2.119	8.683	1.00	78.78
ATOM	185	CE	ARG	A	24	-21.576	-1.972	9.373	1.00	80.11
ATOM	186	NH1	ARG	A	24	-22.483	-1.049	9.068	1.00	80.78
ATOM	187	NH2	ARG	A	24	-22.251	-0.188	8.084	1.00	81.08
ATOM	188	ARG	A	24	-23.623	-0.988	9.744	1.00	81.03	
ATOM	189	C	ARG	A	24	-18.102	-5.919	8.655	1.00	72.74
ATOM	190	O	ARG	A	24	-19.099	-5.940	7.932	1.00	73.15
ATOM	191	N	PRO	A	25	-17.659	-7.021	9.280	1.00	71.00
ATOM	192	CD	PRO	A	25	-16.401	-7.195	10.026	1.00	70.86
ATOM	193	CA	PRO	A	25	-18.367	-8.297	9.129	1.00	69.14
ATOM	194	CB	PRO	A	25	-17.526	-9.256	9.967	1.00	69.82
ATOM	195	CG	PRO	A	25	-16.138	-8.670	9.855	1.00	70.46
ATOM	196	C	PRO	A	25	-19.787	-8.152	9.673	1.00	67.21
ATOM	197	O	PRO	A	25	-19.964	-7.852	10.852	1.00	67.34
ATOM	198	N	THR	A	26	-20.794	-8.355	8.825	1.00	64.60
ATOM	199	CA	THR	A	26	-22.184	-8.218	9.265	1.00	61.62
ATOM	200	CB	THR	A	26	-23.179	-8.457	8.100	1.00	62.41
ATOM	201	OG1	THR	A	26	-22.829	-7.625	6.986	1.00	62.97
ATOM	202	CG2	THR	A	26	-24.598	-8.102	8.535	1.00	58.62
ATOM	203	C	THR	A	26	-22.487	-9.199	10.399	1.00	58.71
ATOM	204	O	THR	A	26	-21.891	-9.105	11.474	1.00	54.49
ATOM	205	N	LEU	A	27	-23.413	-10.128	10.167	1.00	49.96
ATOM	206	CA	LEU	A	27	-23.766	-11.123	11.177	1.00	50.45
ATOM	207	CB	LEU	A	27	-24.522	-12.298	10.546	1.00	50.99
ATOM	208	CG	LEU	A	27	-25.845	-12.037	9.828	1.00	51.87
ATOM	209	CD1	LEU	A	27	-25.611	-11.122	8.637	1.00	51.62
ATOM	210	CD2	LEU	A	2					

Figure 1 (continued 3)

[illegible]

ATOM	366	C	LEU	A	49	-24.325	-15.305					
ATOM	367	O	LEU	A	49	-25.268	-15.928	1.067	1.00	20.63		
ATOM	368	N	GLU	A	50	-23.484	-14.575	0.566	1.00	24.28		
ATOM	369	CA	GLU	A	50	-23.652	-14.494	0.346	1.00	19.18		
ATOM	370	CB	GLU	A	50	-23.243	-13.110	-1.097	1.00	19.11		
ATOM	371	CG	GLU	A	50	-23.515	-12.896	-1.610	1.00	21.43		
ATOM	372	CD	GLU	A	50	-23.235	-11.458	-3.113	1.00	27.31		
ATOM	373	OE1	GLU	A	50	-22.085	-10.968	-3.604	1.00	28.85		
ATOM	374	OE2	GLU	A	50	-24.168	-10.822	-3.454	1.00	31.33		
ATOM	375	C	GLU	A	50	-22.787	-15.559	-4.172	1.00	31.83		
ATOM	376	O	GLU	A	50	-23.166	-16.124	-1.758	1.00	20.12		
ATOM	377	N	MET	A	51	-21.651	-15.846	-2.786	1.00	19.05		
ATOM	378	CA	MET	A	51	-20.698	-16.832	-1.127	1.00	18.26		
ATOM	379	CB	MET	A	51	-19.643	-16.116	-1.670	1.00	18.26		
ATOM	380	CG	MET	A	51	-18.947	-15.032	-2.504	1.00	19.67		
ATOM	381	SD	MET	A	51	-18.086	-14.041	-1.780	1.00	22.10		
ATOM	382	CE	MET	A	51	-16.514	-14.275	-2.993	1.00	25.8		
ATOM	383	C	MET	A	51	-20.053	-17.576	-2.397	1.00	27.36		
ATOM	384	N	MET	A	51	-20.102	-17.129	-0.525	1.00	18.84		
ATOM	385	N	GLU	A	52	-19.428	-18.699	0.634	1.00	18.64		
ATOM	386	CA	GLU	A	52	-18.839	-19.572	-0.853	1.00	16.68		
ATOM	387	CB	GLU	A	52	-19.901	-20.637	0.152	1.00	19.13		
ATOM	388	CG	GLU	A	52	-19.554	-21.806	0.452	1.00	22.65		
ATOM	389	CD	GLU	A	52	-20.803	-22.623	1.323	1.00	32.13		
ATOM	390	OE1	GLU	A	52	-20.682	-23.671	1.650	1.00	34.31		
ATOM	391	OE2	GLU	A	52	-21.913	-22.211	2.325	1.00	38.54		
ATOM	392	C	GLU	A	52	-17.595	-20.188	1.235	1.00	36.05		
ATOM	393	N	GLU	A	52	-17.555	-20.488	-0.449	1.00	18.25		
ATOM	394	O	MET	A	53	-16.584	-20.356	-1.639	1.00	17.91		
ATOM	395	CA	MET	A	53	-15.339	-20.955	0.377	1.00	18.60		
ATOM	396	CB	MET	A	53	-14.202	-19.930	-0.074	1.00	17.33		
ATOM	397	CG	MET	A	53	-12.851	-20.502	-0.036	1.00	21.43		
ATOM	398	SD	MET	A	53	-12.771	-20.914	-0.484	1.00	26.15		
ATOM	399	CE	MET	A	53	-12.410	-19.257	-2.256	1.00	32.73		
ATOM	400	C	MET	A	53	-15.051	-22.112	-2.959	1.00	30.62		
ATOM	401	O	MET	A	53	-15.069	-21.933	0.886	1.00	17.68		
ATOM	402	N	VAL	A	54	-14.786	-23.294	2.102	1.00	17.40		
ATOM	403	CA	VAL	A	54	-14.507	-24.468	0.338	1.00	15.12		
ATOM	404	CB	VAL	A	54	-15.508	-25.612	1.162	1.00	16.82		
ATOM	405	CG1	VAL	A	54	-15.224	-26.754	0.914	1.00	17.64		
ATOM	406	CG2	VAL	A	54	-16.959	-25.117					

Figure 1 (continued 5)

[illegible][illegible]

[illegible]

Figure 1 (continued 7)

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Figure 1 (continued 8)

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Figure 1 (continued 9)

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Figure 1. (continued 10)

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Figure 1. (continued 11)

Figure 1 (continued 12)

[illegible]

Figure 1 (continued 13)

ATOM	1266	CB	GLU	A	163	-21.892	-18.717	-27.287	1.00	21.73	A
ATOM	1267	CD	GLU	A	163	-22.630	-18.615	-28.630	1.00	25.04	A
ATOM	1268	CG	GLU	A	163	-22.892	-17.188	-29.043	1.00	28.71	A
ATOM	1269	OE1	GLU	A	163	-22.046	-16.326	-28.755	1.00	29.00	A
ATOM	1270	OE2	GLU	A	163	-23.937	-16.925	-29.672	1.00	33.20	A
ATOM	1271	C	GLU	A	163	-20.857	-20.965	-27.717	1.00	20.58	A
ATOM	1272	O	GLY	A	164	-19.670	-20.671	-27.849	1.00	19.51	A
ATOM	1273	N	GLY	A	164	-21.427	-21.985	-28.336	1.00	21.25	A
ATOM	1274	CA	GLY	A	164	-20.643	-22.834	-29.208	1.00	23.06	A
ATOM	1275	C	GLY	A	164	-19.570	-23.516	-28.381	1.00	22.55	A
ATOM	1276	O	GLY	A	164	-19.860	-24.269	-27.441	1.00	23.22	A
ATOM	1277	N	GLU	A	165	-18.323	-23.232	-28.699	1.00	22.46	A
ATOM	1278	CA	GLU	A	165	-17.233	-23.835	-27.965	1.00	21.86	A
ATOM	1279	CB	GLU	A	165	-16.276	-24.498	-28.948	1.00	26.05	A
ATOM	1280	CG	GLU	A	165	-15.133	-25.183	-28.299	1.00	31.89	A
ATOM	1281	CD	GLU	A	165	-13.996	-25.386	-29.268	1.00	32.82	A
ATOM	1282	OE1	GLU	A	165	-14.228	-26.054	-30.316	1.00	35.85	A
ATOM	1283	OE2	GLU	A	165	-12.891	-24.872	-28.983	1.00	32.38	A
ATOM	1284	C	GLU	A	165	-16.492	-22.792	-27.122	1.00	20.54	A
ATOM	1285	O	GLU	A	165	-15.403	-23.031	-26.629	1.00	21.57	A
ATOM	1286	N	GLU	A	166	-17.101	-21.632	-26.932	1.00	18.84	A
ATOM	1287	CA	GLU	A	166	-16.419	-20.588	-26.183	1.00	18.69	A
ATOM	1288	CB	GLU	A	166	-16.291	-19.332	-27.036	1.00	20.53	A
ATOM	1289	CG	GLU	A	166	-15.371	-19.476	-28.244	1.00	25.65	A
ATOM	1290	CD	GLU	A	166	-15.124	-18.128	-28.875	1.00	29.36	A
ATOM	1291	OE1	GLU	A	166	-16.106	-17.495	-29.317	1.00	29.76	A
ATOM	1292	OE2	GLU	A	166	-13.953	-17.697	-28.911	1.00	32.95	A
ATOM	1293	C	GLU	A	166	-17.075	-20.149	-24.882	1.00	16.09	A
ATOM	1294	O	LEU	A	167	-18.281	-20.299	-24.699	1.00	17.27	A
ATOM	1295	N	LEU	A	167	-16.226	-19.667	-23.984	1.00	16.29	A
ATOM	1296	CA	LEU	A	167	-16.685	-19.074	-22.722	1.00	14.08	A
ATOM	1297	CB	LEU	A	167	-15.916	-19.586	-21.510	1.00	14.28	A
ATOM	1298	CG	LEU	A	167	-16.345	-18.898	-20.199	1.00	15.20	A
ATOM	1299	CD1	LEU	A	167	-17.852	-19.118	-19.991	1.00	15.60	A
ATOM	1300	CD2	LEU	A	167	-15.572	-19.425	-18.995	1.00	14.38	A
ATOM	1301	C	LEU	A	167	-16.356	-17.589	-22.956	1.00	14.90	A
ATOM	1302	O	LEU	A	167	-15.249	-17.243	-23.413	1.00	13.15	A
ATOM	1303	N	ARG	A	168	-17.314	-16.720	-22.632	1.00	13.65	A
ATOM	1304	CA	ARG	A	168	-17.142	-15.283	-22.858	1.00	14.89	A
ATOM	1305	CB	ARG	A	168	-18.109	-14.851	-23.974	1.00	14.54	A
ATOM	1306	CG	ARG	A	168	-18.286	-13.333	-24.147	1.00	16.30	A
ATOM	1307	CD	ARG	A	168	-19.316	-13.059	-25.217	1.00	19.44	A
ATOM	1308	NE	ARG	A	168	-18.918	-13.676	-26.473	1.00	21.39	A
ATOM	1309	CZ	ARG	A	168	-19.627	-14.584	-27.139	1.00	22.67	A
ATOM	1310	NH1	ARG	A	168	-20.793	-15.006	-26.690	1.00	25.38	A
ATOM	1311	NH2	ARG	A	168	-19.147	-15.073	-28.265	1.00	13.95	A
ATOM	1312	C	ARG	A	168	-17.509	-14.523	-21.605	1.00	14.10	A
ATOM	1313	O	ARG	A	168	-18.425	-14.932	-20.873	1.00	12.43	A
ATOM	1314	N	THR	A	169	-16.794	-13.431	-21.351	1.00	10.45	A
ATOM	1315	CA	THR	A	169	-17.153	-12.587	-20.230	1.00	12.78	A
ATOM	1316	CB	THR	A	169	-16.053	-12.425	-19.186	1.00	14.14	A
ATOM	1317	OG1	THR	A	169	-14.844	-11.981	-19.830	1.00	11.68	A
ATOM	1318	CG2	THR	A	169	-15.808	-13.743	-18.422	1.00	11.09	A
ATOM	1319	C	THR	A	169	-17.469	-11.219	-20.825	1.00	10.97	A
ATOM	1320	O	THR	A	169	-16.932	-10.824	-21.853	1.00	10.12	A
ATOM	1321	N	VAL	A	170	-18.421	-10.537	-20.198	1.00	10.95	A
ATOM	1322	CA	VAL	A	170	-18.803	-9.205	-20.645	1.00	10.17	A
ATOM	1323	CB	VAL	A	170	-20.166	-9.186	-21.384	1.00	11.54	A
ATOM	1324	CG1	VAL	A	170	-20.344	-7.769	-22.015	1.00	13.32	A
ATOM	1325	CG2	VAL	A	170	-20.197	-10.227	-22.491	1.00	10.18	A
ATOM	1326	C	VAL	A	170	-18.967	-8.359	-19.376	1.00	13.17	A
ATOM	1327	O	VAL	A	170	-19.500	-8.824	-18.361	1.00	11.08	A
ATOM	1328	N	ALA	A	171	-18.471	-7.118	-19.426	1.00	10.99	A
ATOM	1329	CA	ALA	A	171	-18.650	-6.212	-18.310	1.00	12.41	A
ATOM	1330	CB	ALA	A	171	-17.451	-6.224	-17.401	1.00	12.83	A
ATOM	1331	C	ALA	A	171	-18.898	-4.807	-18.854	1.00	13.33	A
ATOM	1332	O	ALA	A	171	-18.353	-4.409	-19.875	1.00	11.14	A
ATOM	1333	N	THR	A	172	-19.788	-4.091	-18.193	1.00	12.97	A
ATOM	1334	CA	THR	A	172	-20.092	-2.723	-18.627	1.00	16.11	A
ATOM	1335	CB	THR	A	172	-21.046	-2.669	-19.850	1.00	15.65	A
ATOM	1336	OG1	THR	A	172	-21.222	-1.284	-20.236	1.00	15.53	A
ATOM	1337	CG2	THR	A	172	-22.435	-3.271	-19.520	1.00	13.38	A
ATOM	1338	C	THR	A	172	-20.697	-1.934	-17.486	1.00	13.88	A
ATOM	1339	O	THR	A	172	-21.347	-2.484	-16.592	1.00	13.39	A
ATOM	1340	N	ASP	A	173	-20.455	-0.624	-17.525	1.00	15.62	A
ATOM	1341	CA	ASP	A	173	-20.994	0.264	-16.494	1.00	16.03	A
ATOM	1342	CB	ASP	A	173	-19.864	0.956	-15.731	1.00	16.32	A
ATOM	1343	CG	ASP	A	173	-18.990	1.833	-16.625	1.00	15.70	A
ATOM	1344	OD1	ASP	A	173	-19.273	1.986	-17.831	1.00	18.84	A
ATOM	1345	OD2	ASP	A	173	-18.005	2.370	-16.079	1.00	16.64	A
ATOM	1346	C	ASP	A	173	-21.867	1.310	-17.164	1.00	19.53	A
ATOM	1347	O	ASP	A	173	-22.214	2.322	-16.530	1.00	16.21	A
ATOM	1348	N	GLY	A	174	-22.187	1.083	-18.436	1.00	18.97	A
ATOM	1349	CA	GLY	A	174	-23.039	2.014	-19.977	1.00	19.77	A
ATOM	1350	C	GLY	A	174	-22.302	3.071	-20.860	1.00	21.66	A
ATOM	1351	O	GLY	A	174	-22.884	3.728	-19.655	1.00	18.37	A
ATOM	1352	N	HIS	A	175	-21.023	3.258	-20.370	1.00	19.07	A
ATOM	1353	CA	HIS	A	175	-20.182	4.210	-19.384	1.00	21.34	A
ATOM	1354	CB	HIS	A	175	-19.434	5.082	-17.305	1.00	31.83	A
ATOM	1355	CG	HIS	A	175	-20.339	5.944	-18.126	1.00	30.90	A
ATOM	1356	CD2	HIS	A	175	-20.783	5.827	-17.111	1.00	34.27	A
ATOM	1357	ND1	HIS	A	175	-21.007	7.017	-21.254	1.00	17.40	A
ATOM	1358	CE1	HIS	A	175	-21.828	7.524	-22.340	1.00	18.83	A
ATOM	1359	NE2	HIS	A	175	-21.713	6.820	-20.755	1.00	15.38	A
ATOM	1360	C	HIS	A	175	-19.189	3.501	-21.529	1.00	14.64	A
ATOM	1361	O	HIS	A	175	-18.861	3.970	-21.167	1.00	15.67	A
ATOM	1362	N	ARG	A	176	-18.663	2.385	-19.734	1.00		A
ATOM	1363	CA	ARG	A	176	-17.713	1.611		1.00		A
ATOM	1364	CB	ARG	A	176	-16.248	1.967		1.00		A
ATOM	1365	CG	ARG	A	176	-15.987	2.385		1.00		A

Figure 1 (continued 14)

Figure 1 (continued 15)

ATOM	1966	OD2	ASP	A	253	-15.400	4.962	-42.784	1.00	41.27	A
ATOM	1967	C	ASP	A	253	-13.467	2.586	-40.870	1.00	30.28	A
ATOM	1968	O	ASP	A	253	-12.578	2.126	-41.600	1.00	31.43	A
ATOM	1969	N	LYS	A	254	-13.277	3.606	-40.039	1.00	27.06	A
ATOM	1970	CA	LYS	A	254	-11.991	4.285	-39.932	1.00	24.92	A
ATOM	1971	CB	LYS	A	254	-12.232	5.728	-39.494	1.00	24.91	A
ATOM	1972	CG	LYS	A	254	-13.148	6.522	-40.421	1.00	27.11	A
ATOM	1973	CD	LYS	A	254	-13.379	7.918	-39.844	1.00	29.21	A
ATOM	1974	CE	LYS	A	254	-14.184	8.777	-40.825	1.00	32.00	A
ATOM	1975	NZ	LYS	A	254	-15.470	8.129	-41.185	1.00	34.43	A
ATOM	1976	C	LYS	A	254	-11.094	3.553	-38.930	1.00	22.15	A
ATOM	1977	O	LYS	A	254	-11.328	3.610	-37.730	1.00	22.88	A
ATOM	1978	N	HIS	A	255	-10.067	2.884	-39.434	1.00	21.10	A
ATOM	1979	CA	HIS	A	255	-9.165	2.101	-38.598	1.00	21.30	A
ATOM	1980	CB	HIS	A	255	-8.939	0.721	-39.214	1.00	24.75	A
ATOM	1981	CG	HIS	A	255	-10.171	-0.127	-39.294	1.00	26.36	A
ATOM	1982	CD2	HIS	A	255	-10.391	-1.313	-39.905	1.00	28.26	A
ATOM	1983	ND1	HIS	A	255	-11.359	0.219	-38.684	1.00	29.22	A
ATOM	1984	CE1	HIS	A	255	-12.261	-0.718	-38.922	1.00	29.44	A
ATOM	1985	NE2	HIS	A	255	-11.699	-1.658	-39.660	1.00	31.29	A
ATOM	1986	C	HIS	A	255	-7.798	2.727	-38.381	1.00	20.47	A
ATOM	1987	O	HIS	A	255	-7.045	2.966	-39.331	1.00	19.05	A
ATOM	1988	N	LEU	A	256	-7.449	2.930	-37.120	1.00	18.43	A
ATOM	1989	CA	LEU	A	256	-6.148	3.491	-36.778	1.00	18.02	A
ATOM	1990	CB	LEU	A	256	-6.351	4.753	-35.927	1.00	19.89	A
ATOM	1991	CG	LEU	A	256	-5.142	5.472	-35.324	1.00	22.32	A
ATOM	1992	CD1	LEU	A	256	-5.493	6.944	-35.096	1.00	24.64	A
ATOM	1993	CD2	LEU	A	256	-4.737	4.798	-34.007	1.00	23.40	A
ATOM	1994	C	LEU	A	256	-5.368	2.452	-35.962	1.00	18.20	A
ATOM	1995	O	LEU	A	256	-5.921	1.857	-35.042	1.00	17.77	A
ATOM	1996	N	GLU	A	257	-4.099	2.224	-36.298	1.00	16.89	A
ATOM	1997	CA	GLU	A	257	-3.295	1.292	-35.505	1.00	17.61	A
ATOM	1998	CB	GLU	A	257	-2.702	0.186	-36.378	1.00	19.65	A
ATOM	1999	CG	GLU	A	257	-1.850	-0.790	-35.585	1.00	25.47	A
ATOM	2000	CD	GLU	A	257	-1.391	-1.990	-36.398	1.00	28.58	A
ATOM	2001	OE1	GLU	A	257	-0.339	-2.592	-36.024	1.00	30.83	A
ATOM	2002	OE2	GLU	A	257	-2.089	-2.333	-37.394	1.00	26.86	A
ATOM	2003	C	GLU	A	257	-2.182	-2.113	-34.861	1.00	17.45	A
ATOM	2004	N	ALA	A	258	-1.570	2.963	-35.515	1.00	16.51	A
ATOM	2005	CA	ALA	A	258	-1.932	1.863	-33.579	1.00	17.17	A
ATOM	2006	CB	ALA	A	258	-0.906	2.593	-32.830	1.00	17.02	A
ATOM	2007	C	ALA	A	258	-1.584	3.719	-32.020	1.00	18.18	A
ATOM	2008	O	ALA	A	258	-0.172	1.666	-31.864	1.00	18.03	A
ATOM	2009	N	GLY	A	259	-0.738	0.663	-31.398	1.00	17.35	A
ATOM	2010	CA	GLY	A	259	1.085	2.001	-31.571	1.00	16.83	A
ATOM	2011	C	GLY	A	259	1.860	1.248	-30.598	1.00	16.02	A
ATOM	2012	O	GLY	A	259	1.145	1.382	-29.257	1.00	16.37	A
ATOM	2013	N	CYS	A	260	0.829	2.476	-28.834	1.00	15.32	A
ATOM	2014	CA	CYS	A	260	0.894	0.270	-28.576	1.00	14.83	A
ATOM	2015	CB	CYS	A	260	0.143	0.338	-27.323	1.00	14.73	A
ATOM	2016	SG	CYS	A	260	-0.107	-1.069	-26.807	1.00	13.90	A
ATOM	2017	C	CYS	A	260	-1.234	-1.099	-25.368	1.00	18.12	A
ATOM	2018	O	CYS	A	260	0.806	1.179	-26.253	1.00	14.83	A
ATOM	2019	N	ASP	A	261	0.159	2.047	-25.640	1.00	15.46	A
ATOM	2020	CA	ASP	A	261	2.096	0.921	-26.017	1.00	15.27	A
ATOM	2021	CB	ASP	A	261	2.834	1.655	-24.977	1.00	17.33	A
ATOM	2022	CG	ASP	A	261	4.276	1.123	-24.801	1.00	18.87	A
ATOM	2023	CD	ASP	A	261	5.188	2.109	-24.002	1.00	25.56	A
ATOM	2024	OD1	ASP	A	261	5.948	2.946	-24.607	1.00	27.19	A
ATOM	2025	OD2	ASP	A	261	5.128	2.056	-22.758	1.00	23.92	A
ATOM	2026	C	ASP	A	261	2.924	3.126	-25.321	1.00	15.20	A
ATOM	2027	O	ASP	A	261	2.689	3.977	-24.457	1.00	16.28	A
ATOM	2028	N	LEU	A	262	3.263	3.435	-26.566	1.00	15.05	A
ATOM	2029	CA	LEU	A	262	3.379	4.835	-26.940	1.00	14.87	A
ATOM	2030	CB	LEU	A	262	3.900	4.980	-28.365	1.00	16.84	A
ATOM	2031	CG	LEU	A	262	5.392	4.695	-28.564	1.00	19.33	A
ATOM	2032	CD1	LEU	A	262	5.705	4.835	-30.069	1.00	20.64	A
ATOM	2033	CD2	LEU	A	262	6.233	5.673	-27.721	1.00	19.45	A
ATOM	2034	C	LEU	A	262	2.041	5.563	-26.782	1.00	15.27	A
ATOM	2035	O	LEU	A	262	2.003	6.712	-26.332	1.00	15.81	A
ATOM	2036	N	LEU	A	263	0.949	4.912	-27.161	1.00	13.33	A
ATOM	2037	CA	LEU	A	263	-0.352	5.560	-26.991	1.00	13.53	A
ATOM	2038	CB	LEU	A	263	-1.447	4.721	-27.673	1.00	13.61	A
ATOM	2039	CG	LEU	A	263	-2.885	5.243	-27.627	1.00	16.53	A
ATOM	2040	CD1	LEU	A	263	-2.965	6.612	-28.293	1.00	17.32	A
ATOM	2041	CD2	LEU	A	263	-3.785	4.257	-28.319	1.00	15.91	A
ATOM	2042	C	LEU	A	263	-0.658	5.736	-25.491	1.00	14.38	A
ATOM	2043	O	LEU	A	263	-1.177	6.774	-25.064	1.00	13.47	A
ATOM	2044	N	LYS	A	264	-0.372	4.719	-24.680	1.00	13.04	A
ATOM	2045	CA	LYS	A	264	-0.655	4.778	-23.255	1.00	14.11	A
ATOM	2046	CB	LYS	A	264	-0.299	3.420	-22.644	1.00	15.66	A
ATOM	2047	CG	LYS	A	264	-0.539	3.304	-21.166	1.00	22.39	A
ATOM	2048	CD	LYS	A	264	-0.002	1.952	-20.693	1.00	25.24	A
ATOM	2049	CE	LYS	A	264	-0.624	0.789	-21.454	1.00	28.82	A
ATOM	2050	NZ	LYS	A	264	-0.186	-0.554	-20.920	1.00	32.53	A
ATOM	2051	C	LYS	A	264	0.110	5.920	-22.559	1.00	13.53	A
ATOM	2052	O	LYS	A	264	-0.474	6.700	-21.798	1.00	13.19	A
ATOM	2053	N	GLN	A	265	1.397	6.058	-22.861	1.00	12.97	A
ATOM	2054	CA	GLN	A	265	2.167	7.097	-22.192	1.00	13.73	A
ATOM	2055	CB	GLN	A	265	3.668	6.889	-22.418	1.00	14.32	A
ATOM	2056	CG	GLN	A	265	4.187	5.506	-21.997	1.00	15.83	A
ATOM	2057	CD	GLN	A	265	3.603	5.004	-20.674	1.00	16.85	A
ATOM	2058	OE1	GLN	A	265	3.288	5.773	-19.777	1.00	18.55	A
ATOM	2059	NE2	GLN	A	265	3.473	3.687	-20.551	1.00	19.72	A
ATOM	2060	C	GLN	A	265	1.789	8.491	-22.685	1.00	13.91	A
ATOM	2061	O	ALA	A	266	1.882	9.454	-21.921	1.00	14.00	A
ATOM	2062	N	ALA	A	266	1.367	8.598	-23.947	1.00	12.99	A
ATOM	2063	CA	ALA	A	266	0.949	9.897	-24.477	1.00	12.33	A
ATOM	2064	CB	ALA	A	266	0.735	9.820	-25.983	1.00	13.59	A
ATOM	2065	C	ALA	A	266	-0.356	10.311	-23.760	1.00	14.35	A

Figure 1 (continued 21)

ATOM	2166	CG	ARG	A	279	-8.186	13.898	-15.146	1.00	23.64
ATOM	2167	CD	ARG	A	279	-6.825	13.215	-14.864	1.00	26.45
ATOM	2168	NE	ARG	A	279	-6.393	13.464	-13.493	1.00	31.51
ATOM	2169	CZ	ARG	A	279	-5.871	14.612	-13.074	1.00	33.69
ATOM	2170	NH1	ARG	A	279	-5.708	15.616	-13.934	1.00	35.31
ATOM	2171	NH2	ARG	A	279	-5.529	14.763	-11.792	1.00	33.02
ATOM	2172	C	ARG	A	279	-10.359	13.458	-18.314	1.00	14.43
ATOM	2173	CON	ARG	A	279	-10.674	12.294	-18.433	1.00	16.83
ATOM	2174	CON	GLY	A	280	-10.222	14.291	-19.333	1.00	14.30
ATOM	2175	CA	GLY	A	280	-10.420	13.855	-20.696	1.00	13.40
ATOM	2176	CON	GLY	A	280	-9.408	14.511	-21.632	1.00	12.18
ATOM	2177	CON	VAL	A	281	-8.837	15.565	-21.311	1.00	13.28
ATOM	2178	CA	VAL	A	281	-9.193	13.896	-22.795	1.00	13.04
ATOM	2179	CB	VAL	A	281	-8.254	14.440	-23.796	1.00	12.38
ATOM	2180	CG1	VAL	A	281	-6.960	13.531	-23.909	1.00	13.51
ATOM	2181	CG2	VAL	A	281	-6.103	13.679	-22.671	1.00	12.12
ATOM	2182	C	VAL	A	281	-7.362	12.090	-24.098	1.00	15.36
ATOM	2183	CO	VAL	A	281	-8.927	14.482	-25.165	1.00	12.53
ATOM	2184	CON	ARG	A	282	-9.866	13.716	-25.457	1.00	13.70
ATOM	2185	N	ARG	A	282	-8.453	15.380	-26.026	1.00	11.74
ATOM	2186	CA	ARG	A	282	-8.987	15.486	-27.364	1.00	13.08
ATOM	2187	CB	ARG	A	282	-9.165	16.947	-27.763	1.00	16.93
ATOM	2188	CG	ARG	A	282	-9.831	17.086	-29.125	1.00	25.93
ATOM	2189	CD	ARG	A	282	-11.067	18.017	-29.069	1.00	33.09
ATOM	2190	NE	ARG	A	282	-11.959	17.716	-27.940	1.00	37.56
ATOM	2191	CZ	ARG	A	282	-13.099	17.025	-28.030	1.00	38.42
ATOM	2192	NH1	ARG	A	282	-13.519	16.552	-29.200	1.00	38.59
ATOM	2193	NH2	ARG	A	282	-13.822	16.805	-26.940	1.00	38.91
ATOM	2194	CON	ARG	A	282	-8.029	14.816	-28.330	1.00	14.43
ATOM	2195	CON	LEU	A	283	-6.815	15.031	-28.216	1.00	16.20
ATOM	2196	CA	LEU	A	283	-8.566	14.022	-29.267	1.00	12.40
ATOM	2197	CB	LEU	A	283	-7.754	13.341	-30.279	1.00	13.04
ATOM	2198	CG	LEU	A	283	-8.052	11.840	-30.387	1.00	14.68
ATOM	2199	CD1	LEU	A	283	-7.290	10.870	-29.488	1.00	17.14
ATOM	2200	CD2	LEU	A	283	-7.408	11.334	-28.017	1.00	18.12
ATOM	2201	C	LEU	A	283	-7.795	9.422	-29.716	1.00	17.55
ATOM	2202	CON	LEU	A	283	-8.039	13.920	-31.638	1.00	15.68
ATOM	2203	CON	TYR	A	284	-9.192	14.041	-32.036	1.00	15.80
ATOM	2204	N	TYR	A	284	-6.988	14.308	-32.338	1.00	13.31
ATOM	2205	CA	TYR	A	284	-7.186	14.776	-33.696	1.00	14.87
ATOM	2206	CB	TYR	A	284	-6.561	16.144	-33.942	1.00	14.87
ATOM	2207	CG	TYR	A	284	-7.063	16.684	-35.265	1.00	16.70
ATOM	2208	CD1	TYR	A	284	-8.155	17.562	-35.312	1.00	18.02
ATOM	2209	CE1	TYR	A	284	-8.709	17.978	-36.542	1.00	19.42
ATOM	2210	CD2	TYR	A	284	-6.532	16.232	-36.466	1.00	16.24
ATOM	2211	CE2	TYR	A	284	-7.077	16.638	-37.685	1.00	18.82
ATOM	2212	CZ	TYR	A	284	-8.165	17.514	-37.713	1.00	19.97
ATOM	2213	OH	TYR	A	284	-6.692	17.919	-38.933	1.00	20.44
ATOM	2214	CON	TYR	A	284	-6.517	13.731	-34.561	1.00	14.90
ATOM	2215	CON	VAL	A	285	-5.293	13.519	-34.503	1.00	15.97
ATOM	2216	N	VAL	A	285	-7.320	13.050	-35.369	1.00	14.02
ATOM	2217	CA	VAL	A	285	-6.768	12.007	-36.209	1.00	14.58
ATOM	2218	CB	VAL	A	285	-7.728	10.797	-36.264	1.00	16.41
ATOM	2219	CG1	VAL	A	285	-7.087	9.678	-37.030	1.00	19.28
ATOM	2220	CG2	VAL	A	285	-8.053	10.335	-34.836	1.00	17.87
ATOM	2221	C	VAL	A	285	-6.566	12.520	-37.615	1.00	13.95
ATOM	2222	CON	VAL	A	285	-7.463	13.109	-38.191	1.00	16.55
ATOM	2223	CON	SER	A	286	-5.376	12.297	-38.168	1.00	13.98
ATOM	2224	CA	SER	A	286	-5.094	12.724	-39.555	1.00	15.23
ATOM	2225	CB	SER	A	286	-4.453	14.129	-39.576	1.00	16.02
ATOM	2226	CG	SER	A	286	-3.165	14.108	-38.984	1.00	15.02
ATOM	2227	CON	SER	A	286	-4.198	11.659	-40.201	1.00	15.90
ATOM	2228	CON	GLU	A	287	-3.859	10.670	-39.558	1.00	16.50
ATOM	2229	N	GLU	A	287	-3.806	11.824	-41.465	1.00	17.09
ATOM	2230	CA	GLU	A	287	-3.006	10.788	-42.132	1.00	20.13
ATOM	2231	CB	GLU	A	287	-2.655	11.245	-43.568	1.00	25.94
ATOM	2232	CG	GLU	A	287	-2.338	10.108	-44.526	1.00	31.11
ATOM	2233	CD	GLU	A	287	-3.594	9.464	-45.178	1.00	33.30
ATOM	2234	OE1	GLU	A	287	-4.753	9.927	-44.995	1.00	36.38
ATOM	2235	OE2	GLU	A	287	-3.410	8.466	-45.909	1.00	17.84
ATOM	2236	C	GLU	A	287	-1.752	10.371	-41.363	1.00	16.79
ATOM	2237	CON	GLU	A	287	-0.845	11.172	-41.104	1.00	15.55
ATOM	2238	N	ASN	A	288	-1.734	9.100	-40.955	1.00	15.15
ATOM	2239	CA	ASN	A	288	-0.648	8.524	-40.188	1.00	18.14
ATOM	2240	CB	ASN	A	288	0.548	8.265	-41.097	1.00	19.57
ATOM	2241	CG	ASN	A	288	0.272	7.178	-42.139	1.00	24.08
ATOM	2242	OD1	ASN	A	288	0.911	7.151	-43.202	1.00	15.66
ATOM	2243	ND2	ASN	A	288	-0.643	6.263	-41.837	1.00	14.72
ATOM	2244	C	ASN	A	288	-0.221	9.333	-38.969	1.00	15.32
ATOM	2245	CON	ASN	A	288	0.933	9.275	-38.548	1.00	12.97
ATOM	2246	CON	GLN	A	289	-1.149	10.083	-38.380	1.00	13.76
ATOM	2247	CA	GLN	A	289	-0.790	10.867	-37.209	1.00	14.58
ATOM	2248	CB	GLN	A	289	-0.352	12.282	-37.632	1.00	15.69
ATOM	2249	CG	GLN	A	289	0.205	13.125	-36.486	1.00	22.72
ATOM	2250	CD	GLN	A	289	0.526	14.534	-36.923	1.00	20.35
ATOM	2251	OE1	GLN	A	289	-0.299	15.468	-36.764	1.00	15.19
ATOM	2252	NE2	GLN	A	289	1.714	14.705	-37.504	1.00	14.85
ATOM	2253	C	GLN	A	289	-1.906	11.022	-36.223	1.00	13.50
ATOM	2254	CON	GLN	A	289	-3.074	11.137	-36.603	1.00	13.78
ATOM	2255	N	LEU	A	290	-1.554	11.041	-34.941	1.00	18.63
ATOM	2256	CA	LEU	A	290	-2.559	11.268	-33.903	1.00	17.72
ATOM	2257	CB	LEU	A	290	-2.738	10.022	-33.017	1.00	17.47
ATOM	2258	CG	LEU	A	290	-3.770	10.099	-31.894	1.00	13.83
ATOM	2259	CD1	LEU	A	290	-5.182	10.294	-32.481	1.00	14.65
ATOM	2260	CD2	LEU	A	290	-3.706	8.818	-31.090	1.00	12.16
ATOM	2261	C	LEU	A	290	-2.022	12.403	-33.039	1.00	13.66
ATOM	2262	CON	LYS	A	291	-0.872	12.377	-32.625	1.00	16.40
ATOM	2263	N	LYS	A	291	-2.864	13.395	-32.755	1.00	
ATOM	2264	CA	LYS	A	291	-2.478	14.486	-31.879	1.00	
ATOM	2265	CB	LYS	A	291	-2.713	15.847	-32.532	1.00	

Figure 1 (continued 23)

[illegible]

Figure 1 (continued 24)

[illegible]

Figure 1 (continued 25)

[illegible]

Figure 1 (continued 26)

ATOM	2566	O	ASN	A	329	-3.353	-3.984	-19.177	1.00	20.96
ATOM	2567	N	ALA	A	330	-5.347	-3.282	-19.966	1.00	18.19
ATOM	2568	CA	ALA	A	330	-5.893	-4.635	-20.059	1.00	20.30
ATOM	2570	C	ALA	A	330	-7.444	-4.597	-20.070	1.00	20.07
ATOM	2571	O	ALA	A	330	-5.385	-5.363	-21.304	1.00	20.84
ATOM	2572	N	LEU	A	331	-5.261	-6.601	-21.312	1.00	21.96
ATOM	2573	CA	LEU	A	331	-5.092	-4.614	-22.365	1.00	20.51
ATOM	2574	CB	LEU	A	331	-4.607	-5.238	-23.606	1.00	22.56
ATOM	2575	CG	LEU	A	331	-4.857	-4.311	-24.807	1.00	19.58
ATOM	2576	CD1	LEU	A	331	-6.319	-4.242	-25.284	1.00	20.93
ATOM	2577	CD2	LEU	A	331	-6.493	-3.076	-26.290	1.00	20.46
ATOM	2578	C	LEU	A	331	-6.749	-5.570	-25.905	1.00	19.08
ATOM	2579	O	LEU	A	331	-3.127	-5.621	-23.508	1.00	25.46
ATOM	2580	N	LYS	A	332	-2.742	-6.688	-23.998	1.00	27.06
ATOM	2581	CA	LYS	A	332	-2.313	-4.753	-22.903	1.00	26.68
ATOM	2582	CB	LYS	A	332	-0.877	-5.002	-22.724	1.00	28.23
ATOM	2583	CG	LYS	A	332	-0.651	-5.661	-21.356	1.00	29.27
ATOM	2584	CD	LYS	A	332	-1.401	-6.966	-21.184	1.00	29.90
ATOM	2585	CE	LYS	A	332	-1.468	-7.412	-19.728	1.00	32.09
ATOM	2586	NZ	LYS	A	332	-2.173	-8.745	-19.658	1.00	32.35
ATOM	2587	C	LYS	A	332	-2.345	-9.225	-18.268	1.00	35.40
ATOM	2588	O	LYS	A	332	-0.266	-5.853	-23.855	1.00	27.53
ATOM	2589	N	CYS	A	333	0.361	-6.884	-23.618	1.00	31.18
ATOM	2590	CA	CYS	A	333	-0.484	-5.404	-25.087	1.00	25.22
ATOM	2591	CB	CYS	A	333	0.010	-6.074	-26.301	1.00	21.25
ATOM	2592	SG	CYS	A	333	-1.158	-6.522	-27.166	1.00	19.35
ATOM	2593	C	CYS	A	333	-2.257	-5.131	-27.559	1.00	20.24
ATOM	2594	O	CYS	A	333	0.878	-5.087	-27.069	1.00	20.62
ATOM	2595	N	GLU	A	334	1.047	-3.966	-26.640	1.00	20.60
ATOM	2596	CA	GLU	A	334	1.422	-5.490	-28.218	1.00	19.42
ATOM	2597	CB	GLU	A	334	2.317	-4.604	-28.956	1.00	19.82
ATOM	2598	CG	GLU	A	334	3.102	-5.421	-29.998	1.00	21.89
ATOM	2599	CD	GLU	A	334	4.169	-4.662	-30.765	1.00	27.12
ATOM	2600	OE1	GLU	A	334	5.320	-4.181	-29.882	1.00	29.45
ATOM	2601	OE2	GLU	A	334	5.657	-4.863	-28.890	1.00	32.60
ATOM	2602	C	GLU	A	334	5.902	-3.121	-30.198	1.00	32.88
ATOM	2603	O	GLU	A	334	1.625	-3.429	-29.636	1.00	16.58
ATOM	2604	N	ASN	A	335	2.060	-2.292	-29.474	1.00	16.78
ATOM	2605	CA	ASN	A	335	0.576	-3.704	-30.402	1.00	16.51
ATOM	2606	CB	ASN	A	335	-0.146	-2.651	-31.136	1.00	15.36
ATOM	2607	CG	ASN	A	335	0.089	-2.780	-32.646	1.00	18.00
ATOM	2608	OD1	ASN	A	335	1.546	-2.690	-33.022	1.00	20.47
ATOM	2609	ND2	ASN	A	335	2.162	-3.672	-33.464	1.00	25.38
ATOM	2610	C	ASN	A	335	2.103	-1.518	-32.867	1.00	18.14
ATOM	2611	O	ASN	A	335	-1.646	-2.792	-30.914	1.00	16.50
ATOM	2612	N	VAL	A	336	-2.167	-3.914	-30.726	1.00	16.59
ATOM	2613	CA	VAL	A	336	-2.327	-1.661	-30.918	1.00	16.20
ATOM	2614	CB	VAL	A	336	-3.764	-1.655	-30.767	1.00	14.76
ATOM	2615	CG1	VAL	A	336	-4.247	-0.853	-29.501	1.00	16.01
ATOM	2616	CG2	VAL	A	336	-3.681	-1.469	-28.239	1.00	19.32
ATOM	2617	C	VAL	A	336	-3.854	-0.619	-29.614	1.00	18.64
ATOM	2618	O	VAL	A	336	-4.390	-1.040	-31.993	1.00	16.20
ATOM	2619	N	ARG	A	337	-3.766	-0.257	-32.719	1.00	15.92
ATOM	2620	CA	ARG	A	337	-5.631	-1.422	-32.238	1.00	16.08
ATOM	2621	CB	ARG	A	337	-6.391	-0.860	-33.330	1.00	17.59
ATOM	2622	CG	ARG	A	337	-6.879	-1.961	-34.281	1.00	20.37
ATOM	2623	CD	ARG	A	337	-7.779	-1.445	-35.423	1.00	24.09
ATOM	2624	NE	ARG	A	337	-8.161	-2.499	-36.481	1.00	26.96
ATOM	2625	CZ	ARG	A	337	-6.983	-3.165	-37.020	1.00	29.58
ATOM	2626	NH1	ARG	A	337	-6.568	-4.369	-36.628	1.00	30.93
ATOM	2627	NH2	ARG	A	337	-7.254	-5.040	-35.706	1.00	33.27
ATOM	2628	C	ARG	A	337	-5.446	-4.880	-37.124	1.00	31.58
ATOM	2629	O	ARG	A	337	-7.602	-0.160	-32.741	1.00	17.83
ATOM	2630	N	MET	A	338	-8.342	-0.739	-31.919	1.00	17.99
ATOM	2631	CA	MET	A	338	-7.803	1.092	-33.154	1.00	16.35
ATOM	2632	CB	MET	A	338	-8.976	1.881	-32.731	1.00	17.54
ATOM	2633	CG	MET	A	338	-8.561	3.298	-32.322	1.00	19.03
ATOM	2634	SD	MET	A	338	-7.696	3.343	-31.067	1.00	22.98
ATOM	2635	CE	MET	A	338	-7.251	5.013	-30.485	1.00	28.14
ATOM	2636	C	MET	A	338	-8.672	5.347	-29.411	1.00	24.78
ATOM	2637	O	MET	A	338	-9.867	1.943	-33.963	1.00	17.28
ATOM	2638	N	MET	A	339	-9.398	2.321	-35.033	1.00	18.78
ATOM	2639	CA	MET	A	339	-11.144	1.591	-33.825	1.00	17.39
ATOM	2640	CB	MET	A	339	-12.064	1.582	-34.955	1.00	17.39
ATOM	2641	CG	MET	A	339	-12.686	0.180	-35.053	1.00	20.98
ATOM	2642	SD	MET	A	339	-11.628	-0.888	-34.852	1.00	25.07
ATOM	2643	CE	MET	A	339	-12.307	-2.536	-34.442	1.00	30.90
ATOM	2644	C	MET	A	339	-12.758	-2.891	-36.141	1.00	27.62
ATOM	2645	O	MET	A	339	-13.075	2.676	-34.673	1.00	18.45
ATOM	2646	N	LEU	A	340	-13.868	2.596	-33.729	1.00	17.17
ATOM	2647	CA	LEU	A	340	-13.009	3.728	-35.490	1.00	17.41
ATOM	2648	CB	LEU	A	340	-13.853	4.898	-35.313	1.00	19.07
ATOM	2649	CG	LEU	A	340	-12.974	6.150	-35.330	1.00	21.15
ATOM	2650	CD1	LEU	A	340	-11.856	6.140	-34.291	1.00	22.56
ATOM	2651	CD2	LEU	A	340	-10.597	6.765	-34.885	1.00	27.71
ATOM	2652	C	LEU	A	340	-12.321	6.886	-33.043	1.00	24.99
ATOM	2653	O	LEU	A	340	-14.892	5.036	-36.396	1.00	20.06
ATOM	2654	N	THR	A	341	-14.739	4.483	-37.481	1.00	20.26
ATOM	2655	CA	THR	A	341	-15.941	5.783	-36.086	1.00	22.17
ATOM	2656	CB	THR	A	341	-17.029	6.020	-37.026	1.00	25.08
ATOM	2657	CG1	THR	A	341	-18.360	5.576	-36.433	1.00	26.10
ATOM	2658	CG2	THR	A	341	-18.287	4.178	-36.133	1.00	25.61
ATOM	2659	C	THR	A	341	-19.487	5.811	-37.438	1.00	26.42
ATOM	2660	O	THR	A	341	-17.084	7.509	-37.328	1.00	25.45
ATOM	2661	N	ASP	A	342	-16.921	7.922	-38.481	1.00	27.99
ATOM	2662	CA	ASP	A	342	-17.320	8.298	-36.284	1.00	25.19
ATOM	2663	CB	ASP	A	342	-17.367	9.757	-36.381	1.00	24.72
ATOM	2664	CG	ASP	A	342	-18.690	10.235	-37.008	1.00	25.68
ATOM	2665	OD1	ASP	A	342	-19.905	9.816	-36.214	1.00	27.08
ATOM						-19.828	9.819	-34.967	1.00	25.89

Figure 1 (continued 27)

[illegible][illegible]

[illegible]

Figure 1 (continued 29)

ATOM	2866	CD1	PHE	B	3	15.726	25.391	-16.719	1.00	12.95	
ATOM	2867	CD2	PHE	B	3	16.192	23.108	-17.354	1.00	11.17	
ATOM	2868	CE1	PHE	B	3	14.607	24.944	-15.988	1.00	13.10	
ATOM	2869	CE2	PHE	B	3	15.088	22.664	-16.639	1.00	13.73	
ATOM	2870	CZ	PHE	B	3	14.300	23.598	-15.956	1.00	11.90	
ATOM	2871	C	PHE	B	3	17.047	23.862	-20.358	1.00	12.91	
ATOM	2872	O	PHE	B	3	15.870	23.705	-20.657	1.00	14.61	
ATOM	2873	N	THR	B	4	17.981	22.983	-20.677	1.00	12.44	
ATOM	2874	CA	THR	B	4	17.647	21.694	-21.264	1.00	12.80	
ATOM	2875	CB	THR	B	4	18.054	21.570	-22.727	1.00	14.32	
ATOM	2876	OG1	THR	B	4	17.465	22.636	-23.492	1.00	17.57	
ATOM	2877	CG2	THR	B	4	17.564	20.235	-23.258	1.00	15.46	
ATOM	2878	C	THR	B	4	18.437	20.668	-20.440	1.00	14.04	
ATOM	2879	O	THR	B	4	19.658	20.774	-20.291	1.00	14.28	
ATOM	2880	N	VAL	B	5	17.740	19.692	-19.870	1.00	14.07	
ATOM	2881	CA	VAL	B	5	18.377	18.702	-19.003	1.00	14.50	
ATOM	2882	CB	VAL	B	5	18.137	19.055	-17.497	1.00	14.63	
ATOM	2883	CG1	VAL	B	5	18.774	17.995	-16.572	1.00	19.00	
ATOM	2884	CG2	VAL	B	5	18.711	20.379	-17.153	1.00	19.65	
ATOM	2885	C	VAL	B	5	17.841	17.296	-19.293	1.00	16.13	
ATOM	2886	O	VAL	B	5	16.685	17.117	-19.675	1.00	15.26	
ATOM	2887	N	GLU	B	6	18.694	16.294	-19.151	1.00	14.93	
ATOM	2888	CA	GLU	B	6	18.295	14.932	-19.348	1.00	17.40	
ATOM	2889	CB	GLU	B	6	19.563	14.057	-19.314	1.00	24.92	
ATOM	2890	CG	GLU	B	6	19.320	12.568	-19.294	1.00	30.16	
ATOM	2891	CD	GLU	B	6	20.397	11.849	-18.509	1.00	31.47	
ATOM	2892	OE1	GLU	B	6	21.409	11.429	-19.117	1.00	14.96	
ATOM	2893	OE2	GLU	B	6	20.235	11.721	-17.269	1.00	13.59	
ATOM	2894	C	GLU	B	6	17.304	14.577	-18.204	1.00	13.17	
ATOM	2895	O	GLU	B	6	17.478	14.983	-17.044	1.00	13.08	
ATOM	2896	N	ARG	B	7	16.268	13.831	-18.547	1.00	12.64	
ATOM	2897	CA	ARG	B	7	15.235	13.435	-17.595	1.00	11.85	
ATOM	2898	CB	ARG	B	7	14.341	12.368	-18.216	1.00	14.66	
ATOM	2899	CG	ARG	B	7	13.332	11.764	-17.240	1.00	13.57	
ATOM	2900	CD	ARG	B	7	12.547	10.721	-17.988	1.00	17.64	
ATOM	2901	NE	ARG	B	7	11.561	10.026	-17.142	1.00	17.50	
ATOM	2902	CZ	ARG	B	7	11.809	8.942	-16.404	1.00	15.79	
ATOM	2903	NH1	ARG	B	7	13.015	8.381	-16.365	1.00	14.94	
ATOM	2904	NH2	ARG	B	7	10.839	8.391	-15.706	1.00	13.48	
ATOM	2905	C	ARG	B	7	15.748	12.932	-16.243	1.00	15.15	
ATOM	2906	O	ARG	B	7	15.326	13.421	-15.202	1.00	18.15	
ATOM	2907	N	GLU	B	8	16.679	11.981	-16.256	1.00	18.04	
ATOM	2908	CA	GLU	B	8	17.145	11.434	-14.973	1.00	17.91	
ATOM	2909	CB	GLU	B	8	17.861	10.104	-15.238	1.00	19.66	
ATOM	2910	CG	GLU	B	8	16.929	9.035	-15.849	1.00	18.19	
ATOM	2911	CD	GLU	B	8	16.576	9.297	-17.297	1.00	20.48	
ATOM	2912	OE1	GLU	B	8	17.433	9.801	-18.024	1.00	19.63	
ATOM	2913	OE2	GLU	B	8	15.460	8.978	-17.745	1.00	21.28	
ATOM	2914	C	GLU	B	8	17.988	12.368	-14.103	1.00	23.49	
ATOM	2915	O	GLU	B	8	18.056	12.219	-12.878	1.00	25.02	
ATOM	2916	N	HIS	B	9	18.613	13.364	-14.728	1.00	28.09	
ATOM	2917	CA	HIS	B	9	19.426	14.333	-14.008	1.00	26.71	
ATOM	2918	CB	HIS	B	9	20.297	15.041	-15.071	1.00	27.14	
ATOM	2919	CG	HIS	B	9	21.522	15.711	-14.538	1.00	29.19	
ATOM	2920	CD2	HIS	B	9	21.915	17.007	-14.589	1.00	22.99	
ATOM	2921	ND1	HIS	B	9	22.466	15.056	-13.780	1.00	23.60	
ATOM	2922	CE1	HIS	B	9	23.377	15.920	-13.367	1.00	21.72	
ATOM	2923	NE2	HIS	B	9	23.064	17.114	-13.843	1.00	21.01	
ATOM	2924	C	HIS	B	9	18.460	15.284	-13.250	1.00	21.10	
ATOM	2925	O	HIS	B	9	18.789	15.913	-12.229	1.00	19.07	
ATOM	2926	N	LEU	B	10	17.222	15.347	-13.737	1.00	20.85	
ATOM	2927	CA	LEU	B	10	16.202	16.182	-13.157	1.00	22.03	
ATOM	2928	CB	LEU	B	10	15.454	16.876	-14.310	1.00	23.32	
ATOM	2929	CG	LEU	B	10	14.381	17.868	-13.903	1.00	19.50	
ATOM	2930	CD1	LEU	B	10	15.051	19.052	-13.212	1.00	21.06	
ATOM	2931	CD2	LEU	B	10	13.613	18.369	-15.152	1.00	21.78	
ATOM	2932	C	LEU	B	10	15.181	15.513	-12.200	1.00	23.01	
ATOM	2933	O	LEU	B	10	14.732	16.119	-11.216	1.00	26.14	
ATOM	2934	N	LEU	B	11	14.860	14.247	-12.460	1.00	26.14	
ATOM	2935	CA	LEU	B	11	13.848	13.520	-11.718	1.00	21.79	
ATOM	2936	CB	LEU	B	11	13.667	12.159	-12.376	1.00	21.56	
ATOM	2937	CG	LEU	B	11	12.270	11.573	-12.315	1.00	23.82	
ATOM	2938	CD1	LEU	B	11	11.245	12.601	-12.812	1.00	24.71	
ATOM	2939	CD2	LEU	B	11	12.219	10.366	-13.214	1.00	28.61	
ATOM	2940	C	LEU	B	11	13.979	13.363	-10.192	1.00	31.97	
ATOM	2941	O	LEU	B	11	13.053	13.717	-9.453	1.00	36.79	
ATOM	2942	N	LYS	B	12	15.095	12.826	-9.717	1.00	37.65	
ATOM	2943	CA	LYS	B	12	15.250	12.672	-8.267	1.00	39.04	
ATOM	2944	CB	LYS	B	12	16.543	11.923	-7.915	1.00	22.39	
ATOM	2945	CG	LYS	B	12	16.608	11.564	-6.431	1.00	22.26	
ATOM	2946	CD	LYS	B	12	17.856	10.741	-6.085	1.00	20.35	
ATOM	2947	CE	LYS	B	12	17.795	10.213	-4.650	1.00	19.55	
ATOM	2948	NZ	LYS	B	12	17.449	11.262	-3.640	1.00	19.49	
ATOM	2949	C	LYS	B	12	15.224	14.040	-7.576	1.00	19.36	
ATOM	2950	O	LYS	B	12	14.586	14.193	-6.542	1.00	19.86	
ATOM	2951	N	PRO	B	13	15.932	15.052	-8.123	1.00	19.87	
ATOM	2952	CD	PRO	B	13	17.026	15.053	-9.103	1.00	17.95	
ATOM	2953	CA	PRO	B	13	15.855	16.346	-7.434	1.00	18.71	
ATOM	2954	CB	PRO	B	13	16.669	17.272	-8.333	1.00	22.23	
ATOM	2955	CG	PRO	B	13	17.750	16.376	-8.827	1.00	21.65	
ATOM	2956	C	PRO	B	13	14.420	16.838	-7.294	1.00	20.62	
ATOM	2957	O	PRO	B	13	14.041	17.346	-6.250	1.00	18.11	
ATOM	2958	N	LEU	B	14	13.620	16.710	-8.363	1.00	20.79	
ATOM	2959	CA	LEU	B	14	12.231	17.130	-8.294	1.00	22.60	
ATOM	2960	CB	LEU	B	14	11.532	16.907	-9.641	1.00	23.92	
ATOM	2961	CG	LEU	B	14	11.656	17.995	-10.680	1.00		
ATOM	2962	CD1	LEU	B	14	10.975	17.528	-11.993	1.00		
ATOM	2963	CD2	LEU	B	14	11.024	19.287	-10.152	1.00		
ATOM	2964	C	LEU	B	14	11.464	16.390	-7.215	1.00		
ATOM	2965	O	LEU	B	14	10.644	16.963	-6.504	1.00		

Figure 1 (continued 30)

ATOM	2966	N	GLN	B	15	11.720	15.091	-7.121	1.00	24.48	B
ATOM	2967	CA	GLN	B	15	11.053	14.254	-6.149	1.00	25.57	B
ATOM	2968	CB	GLN	B	15	11.481	12.808	-6.340	1.00	28.51	B
ATOM	2969	CG	GLN	B	15	10.827	11.860	-5.383	1.00	32.34	B
ATOM	2970	CD	GLN	B	15	11.261	10.436	-5.657	1.00	35.26	B
ATOM	2971	OE1	GLN	B	15	11.086	9.924	-6.769	1.00	36.87	B
ATOM	2972	NE2	GLN	B	15	11.841	9.789	-4.651	1.00	37.81	B
ATOM	2973	C	GLN	B	15	11.402	14.692	-3.872	1.00	25.12	B
ATOM	2974	O	GLN	B	16	10.546	14.800	-4.746	1.00	24.87	B
ATOM	2975	N	GLN	B	16	12.685	14.941	-4.533	1.00	23.65	B
ATOM	2976	CA	GLN	B	16	13.133	15.374	-3.224	1.00	23.01	B
ATOM	2977	CB	GLN	B	16	14.649	15.351	-3.161	1.00	26.68	B
ATOM	2978	CG	GLN	B	16	15.220	13.938	-3.057	1.00	33.06	B
ATOM	2979	CD	GLN	B	16	15.149	13.363	-1.639	1.00	34.57	B
ATOM	2980	OE1	GLN	B	16	15.499	12.208	-1.417	1.00	36.18	B
ATOM	2981	NE2	GLN	B	16	14.709	14.170	-0.683	1.00	22.25	B
ATOM	2982	C	GLN	B	16	12.640	16.761	-1.657	1.00	21.67	B
ATOM	2983	O	GLN	B	16	12.218	16.966	-3.697	1.00	19.74	B
ATOM	2984	N	VAL	B	17	12.665	17.731	-3.234	1.00	21.71	B
ATOM	2985	CA	VAL	B	17	12.234	19.045	-4.175	1.00	21.43	B
ATOM	2986	CB	VAL	B	17	12.701	20.165	-4.234	1.00	21.95	B
ATOM	2987	CG1	VAL	B	17	14.229	20.161	-5.563	1.00	17.76	B
ATOM	2988	CG2	VAL	B	17	12.098	20.000	-3.002	1.00	21.93	B
ATOM	2989	C	SER	B	18	10.738	19.160	-2.330	1.00	23.73	B
ATOM	2990	O	SER	B	18	10.278	20.075	-3.545	1.00	25.13	B
ATOM	2991	N	SER	B	18	9.993	18.221	-4.502	1.00	25.03	B
ATOM	2992	CA	SER	B	18	8.548	18.205	-5.727	1.00	24.69	B
ATOM	2993	CB	SER	B	18	7.923	17.397	-2.024	1.00	26.98	B
ATOM	2994	CG	SER	B	18	8.075	18.078	-1.660	1.00	27.31	B
ATOM	2995	O	SER	B	18	8.092	17.636	-1.300	1.00	26.53	B
ATOM	2996	N	GLY	B	19	6.926	17.771	-0.012	1.00	27.63	B
ATOM	2997	CA	GLY	B	19	9.017	17.010	0.951	1.00	27.65	B
ATOM	2998	CB	GLY	B	19	8.706	16.413	1.364	1.00	27.01	B
ATOM	2999	CG	GLY	B	19	7.842	17.206	1.351	1.00	28.69	B
ATOM	3000	O	PRO	B	20	6.788	16.717	1.119	1.00	30.14	B
ATOM	3001	N	PRO	B	20	8.265	18.416	2.288	1.00	29.93	B
ATOM	3002	CA	PRO	B	20	9.611	18.974	2.594	1.00	30.20	B
ATOM	3003	CB	PRO	B	20	7.499	19.255	1.436	1.00	30.31	B
ATOM	3004	CG	PRO	B	20	8.462	20.415	1.848	1.00	31.66	B
ATOM	3005	O	PRO	B	20	9.415	20.424	2.650	1.00	32.04	B
ATOM	3006	N	LEU	B	21	6.111	19.744	0.089	1.00	33.35	B
ATOM	3007	CA	LEU	B	21	5.360	20.297	-1.429	1.00	33.56	B
ATOM	3008	CB	LEU	B	21	5.759	19.532	-1.954	1.00	33.69	B
ATOM	3009	CG	LEU	B	21	4.456	19.982	-1.573	1.00	32.31	B
ATOM	3010	O	LEU	B	21	4.506	20.208	0.412	1.00	36.25	B
ATOM	3011	CD1	LEU	B	21	5.187	21.476	0.452	1.00	37.14	B
ATOM	3012	CD2	LEU	B	21	6.657	21.499	0.636	1.00	38.77	B
ATOM	3013	C	LEU	B	21	5.034	21.520	-0.278	1.00	41.62	B
ATOM	3014	O	LEU	B	21	3.331	19.003	-1.348	1.00	42.14	B
ATOM	3015	N	GLY	B	22	3.543	17.799	-0.117	1.00	42.36	B
ATOM	3016	CA	GLY	B	22	2.132	19.540	-1.214	1.00	42.80	B
ATOM	3017	CB	GLY	B	22	0.982	18.707	-1.621	1.00	42.52	B
ATOM	3018	CG	GLY	B	22	0.122	18.423	-2.776	1.00	42.78	B
ATOM	3019	O	GLY	B	22	0.323	19.015	-0.951	1.00	41.15	B
ATOM	3020	N	GLY	B	23	-0.840	17.516	-0.419	1.00	44.69	B
ATOM	3021	CA	GLY	B	23	-1.731	17.170	-0.973	1.00	48.56	B
ATOM	3022	CB	GLY	B	23	-2.597	18.349	-0.831	1.00	55.67	B
ATOM	3023	CG	GLY	B	23	-3.006	18.470	-1.079	1.00	57.36	B
ATOM	3024	O	ARG	B	24	-2.886	19.223	-0.760	1.00	58.66	B
ATOM	3025	N	ARG	B	24	-3.691	20.400	-1.656	1.00	58.21	B
ATOM	3026	CA	ARG	B	24	-5.114	20.240	-0.332	1.00	38.07	B
ATOM	3027	CB	ARG	B	24	-6.032	21.311	0.845	1.00	38.01	B
ATOM	3028	CG	ARG	B	24	-7.337	21.431	-2.565	1.00	34.80	B
ATOM	3029	O	ARG	B	24	-8.207	22.431	-0.601	1.00	32.06	B
ATOM	3030	NH1	ARG	B	24	-7.851	23.690	-1.779	1.00	31.38	B
ATOM	3031	NH2	ARG	B	24	-6.634	24.122	-2.967	1.00	33.86	B
ATOM	3032	C	ARG	B	24	-8.711	24.521	-0.147	1.00	29.51	B
ATOM	3033	O	ARG	B	24	-3.067	21.645	-0.803	1.00	28.23	B
ATOM	3034	N	PRO	B	25	-3.273	21.934	0.996	1.00	28.41	B
ATOM	3035	CA	PRO	B	25	-2.295	22.401	1.565	1.00	27.34	B
ATOM	3036	CB	PRO	B	25	-2.021	22.244	2.861	1.00	28.45	B
ATOM	3037	CG	PRO	B	25	-1.663	23.611	3.717	1.00	31.15	B
ATOM	3038	O	PRO	B	25	-0.820	24.099	3.546	1.00	28.57	B
ATOM	3039	N	PRO	B	25	-1.619	23.646	0.587	1.00	25.70	B
ATOM	3040	CA	PRO	B	25	-2.692	24.634	0.428	1.00	27.11	B
ATOM	3041	CB	PRO	B	25	-3.711	24.864	-1.044	1.00	23.09	B
ATOM	3042	O	THR	B	26	-2.412	25.236	-1.043	1.00	21.25	B
ATOM	3043	N	THR	B	26	-3.285	26.240	0.511	1.00	21.63	B
ATOM	3044	CA	THR	B	26	-2.673	26.762	0.483	1.00	23.04	B
ATOM	3045	CB	THR	B	26	-2.397	25.643	0.895	1.00	24.85	B
ATOM	3046	CG	THR	B	26	-3.626	27.732	-0.160	1.00	24.74	B
ATOM	3047	O	THR	B	26	-3.504	27.389	-2.247	1.00	20.78	B
ATOM	3048	N	LEU	B	27	-4.624	27.893	-2.105	1.00	17.68	B
ATOM	3049	CA	LEU	B	27	-2.426	27.829	-3.443	1.00	18.82	B
ATOM	3050	CB	LEU	B	27	-2.507	28.881	-4.682	1.00	18.71	B
ATOM	3051	CG	LEU	B	27	-1.953	30.195	-5.722	1.00	18.57	B
ATOM	3052	O	LEU	B	27	-2.900	30.896	-5.195	1.00	20.77	B
ATOM	3053	CD1	LEU	B	27	-2.264	32.203	-4.684	1.00	20.10	B
ATOM	3054	CD2	LEU	B	27	-4.270	31.144	-5.114	1.00	18.35	B
ATOM	3055	C	LEU	B	27	-1.718	28.392	-4.230	1.00	18.61	B
ATOM	3056	O	PRO	B	28	-0.775	27.601	-4.241	1.00	17.45	B
ATOM	3057	N	PRO	B	28	-2.084	28.863				B
ATOM	3058	CA	PRO	B	28	-3.104	29.903				B
ATOM	3059	CB	PRO	B	28	-1.413	28.443				B
ATOM	3060	CG	PRO	B	28	-1.917	29.446				B
ATOM	3061	O	PRO	B	28	-3.292	29.834				B
ATOM	3062	N	PRO	B	28	0.110	28.355				B
ATOM	3063	CA	ILE	B	29	0.666	27.322				B
ATOM	3064		ILE	B	29	0.781	29.409				B
ATOM	3065		ILE	B	29	2.257	29.431				B

Figure 1 (continued 31)

ATOM	3066	CB	ILE	B	29	2.810	30.770	-3.637	1.00	19.27
ATOM	3067	CG2	ILE	B	29	2.555	30.812	-2.154	1.00	20.68
ATOM	3068	CG1	ILE	B	29	4.304	30.917	-3.901	1.00	23.27
ATOM	3069	CD1	ILE	B	29	4.653	31.204	-5.338	1.00	22.71
ATOM	3070	C	ILE	B	29	2.880	28.264	-3.502	1.00	15.97
ATOM	3071	O	ILE	B	29	3.957	27.778	-3.907	1.00	14.64
ATOM	3072	N	LEU	B	30	2.218	27.775	-2.452	1.00	16.95
ATOM	3073	CA	LEU	B	30	2.782	26.670	-1.664	1.00	16.78
ATOM	3074	CB	LEU	B	30	2.094	26.575	-0.300	1.00	18.79
ATOM	3075	CG	LEU	B	30	2.283	27.856	0.524	1.00	19.43
ATOM	3076	CD1	LEU	B	30	1.556	27.675	1.859	1.00	19.92
ATOM	3077	CD2	LEU	B	30	3.728	28.159	0.783	1.00	18.87
ATOM	3078	C	LEU	B	30	2.752	25.322	-2.374	1.00	17.78
ATOM	3079	O	LEU	B	30	3.343	24.340	-1.901	1.00	18.71
ATOM	3080	N	GLY	B	31	2.066	25.280	-3.505	1.00	14.09
ATOM	3081	CA	GLY	B	31	1.999	24.068	-4.318	1.00	15.57
ATOM	3082	C	GLY	B	31	2.992	24.160	-5.466	1.00	13.53
ATOM	3083	O	GLY	B	31	3.038	23.269	-6.317	1.00	15.55
ATOM	3084	N	ASN	B	32	3.796	25.200	-5.476	1.00	12.64
ATOM	3085	CA	ASN	B	32	4.767	25.400	-6.551	1.00	12.56
ATOM	3086	CB	ASN	B	32	4.690	26.838	-7.107	1.00	12.94
ATOM	3087	CG	ASN	B	32	3.502	27.045	-8.024	1.00	10.96
ATOM	3088	OD1	ASN	B	32	2.599	26.224	-8.085	1.00	12.20
ATOM	3089	ND2	ASN	B	32	3.523	28.158	-8.771	1.00	13.16
ATOM	3090	C	ASN	B	32	6.178	25.176	-6.075	1.00	14.19
ATOM	3091	O	ASN	B	32	6.481	25.195	-4.868	1.00	14.24
ATOM	3092	N	LEU	B	33	7.050	24.957	-7.052	1.00	13.85
ATOM	3093	CA	LEU	B	33	8.459	24.861	-6.774	1.00	13.97
ATOM	3094	CB	LEU	B	33	9.097	23.641	-7.433	1.00	15.40
ATOM	3095	CG	LEU	B	33	8.586	22.254	-7.072	1.00	17.90
ATOM	3096	CD1	LEU	B	33	9.410	21.226	-7.867	1.00	18.49
ATOM	3097	CD2	LEU	B	33	8.782	22.024	-5.568	1.00	19.70
ATOM	3098	C	LEU	B	33	9.115	26.086	-7.395	1.00	13.05
ATOM	3099	O	LEU	B	33	8.725	26.540	-8.465	1.00	13.07
ATOM	3100	N	LEU	B	34	10.126	26.610	-6.722	1.00	12.75
ATOM	3101	CA	LEU	B	34	10.895	27.732	-7.225	1.00	12.14
ATOM	3102	CB	LEU	B	34	11.510	28.520	-6.056	1.00	13.47
ATOM	3103	CG	LEU	B	34	12.562	29.560	-6.427	1.00	12.92
ATOM	3104	CD1	LEU	B	34	11.973	30.697	-7.293	1.00	14.04
ATOM	3105	CD2	LEU	B	34	13.130	30.156	-5.123	1.00	14.82
ATOM	3106	C	LEU	B	34	12.029	27.176	-8.099	1.00	13.14
ATOM	3107	O	LEU	B	34	12.760	26.275	-7.652	1.00	12.90
ATOM	3108	N	LEU	B	35	12.125	27.651	-9.351	1.00	11.64
ATOM	3109	CA	LEU	B	35	13.187	27.245	-10.291	1.00	11.91
ATOM	3110	CB	LEU	B	35	12.615	26.811	-11.669	1.00	11.42
ATOM	3111	CG	LEU	B	35	12.046	25.413	-11.738	1.00	14.74
ATOM	3112	CD1	LEU	B	35	11.127	25.120	-10.596	1.00	18.38
ATOM	3113	CD2	LEU	B	35	11.288	25.299	-13.074	1.00	15.91
ATOM	3114	C	LEU	B	35	14.071	28.445	-10.542	1.00	13.47
ATOM	3115	O	LEU	B	35	13.573	29.535	-10.900	1.00	14.51
ATOM	3116	N	GLN	B	36	15.376	28.285	-10.350	1.00	13.11
ATOM	3117	CA	GLN	B	36	16.300	29.400	-10.578	1.00	13.83
ATOM	3118	CB	GLN	B	36	16.806	29.935	-9.223	1.00	16.19
ATOM	3119	CG	GLN	B	36	15.726	30.383	-8.281	1.00	16.86
ATOM	3120	CD	GLN	B	36	16.264	30.626	-6.866	1.00	21.22
ATOM	3121	OE1	GLN	B	36	16.232	31.760	-6.363	1.00	25.16
ATOM	3122	NE2	GLN	B	36	16.770	29.570	-6.229	1.00	16.45
ATOM	3123	C	GLN	B	36	17.495	28.935	-11.376	1.00	13.60
ATOM	3124	N	VAL	B	37	18.135	27.952	-10.993	1.00	14.49
ATOM	3125	CA	VAL	B	37	17.810	29.640	-12.474	1.00	11.56
ATOM	3126	CB	VAL	B	37	18.997	29.285	-13.248	1.00	13.61
ATOM	3127	CG1	VAL	B	37	18.731	29.191	-14.777	1.00	12.84
ATOM	3128	CG2	VAL	B	37	20.074	29.020	-15.553	1.00	14.43
ATOM	3129	C	VAL	B	37	17.804	27.985	-15.051	1.00	14.23
ATOM	3130	O	VAL	B	37	19.965	30.435	-13.005	1.00	15.18
ATOM	3131	N	ALA	B	38	19.611	31.603	-13.228	1.00	15.34
ATOM	3132	CA	ALA	B	38	21.139	30.117	-12.472	1.00	15.02
ATOM	3133	CB	ALA	B	38	22.161	31.146	-12.227	1.00	15.51
ATOM	3134	C	ALA	B	38	21.954	31.783	-10.878	1.00	15.09
ATOM	3135	O	ALA	B	38	23.493	30.446	-12.291	1.00	19.33
ATOM	3136	N	ASP	B	39	23.644	29.366	-11.747	1.00	18.26
ATOM	3137	CA	ASP	B	39	24.473	31.060	-12.953	1.00	22.66
ATOM	3138	CB	ASP	B	39	25.765	30.393	-13.153	1.00	26.58
ATOM	3139	CG	ASP	B	39	26.389	29.982	-11.829	1.00	32.37
ATOM	3140	OD1	ASP	B	39	27.184	31.097	-11.201	1.00	36.57
ATOM	3141	OD2	ASP	B	39	28.336	31.328	-11.655	1.00	39.34
ATOM	3142	C	ASP	B	39	26.658	31.756	-10.270	1.00	38.78
ATOM	3143	O	ASP	B	39	25.429	29.150	-13.986	1.00	26.82
ATOM	3144	N	GLY	B	40	24.550	29.189	-14.844	1.00	29.26
ATOM	3145	CA	GLY	B	40	26.080	28.031	-13.733	1.00	26.59
ATOM	3146	C	GLY	B	40	25.759	26.871	-14.539	1.00	23.64
ATOM	3147	O	GLY	B	40	24.910	25.927	-13.730	1.00	19.76
ATOM	3148	N	THR	B	41	25.044	24.723	-13.871	1.00	20.20
ATOM	3149	CA	THR	B	41	24.046	26.498	-12.883	1.00	18.09
ATOM	3150	CB	THR	B	41	23.215	25.701	-11.983	1.00	15.70
ATOM	3151	CG1	THR	B	41	23.684	25.916	-10.551	1.00	16.47
ATOM	3152	CG2	THR	B	41	25.090	25.633	-10.486	1.00	19.61
ATOM	3153	C	THR	B	41	22.918	25.016	-9.549	1.00	17.43
ATOM	3154	O	THR	B	41	21.721	25.988	-11.974	1.00	13.03
ATOM	3155	N	LEU	B	42	21.308	27.129	-11.944	1.00	14.12
ATOM	3156	CA	LEU	B	42	20.924	24.933	-12.005	1.00	13.26
ATOM	3157	CB	LEU	B	42	19.483	25.093	-21.850	1.00	11.94
ATOM	3158	CG	LEU	B	42	18.743	24.061	-12.723	1.00	11.39
ATOM	3159	CD1	LEU	B	42	17.292	23.803	-12.339	1.00	10.89
ATOM	3160	CD2	LEU	B	42	16.422	25.083	-12.504	1.00	13.06
ATOM	3161	C	LEU	B	42	16.760	22.694	-13.241	1.00	12.39
ATOM	3162	O	LEU	B	42	19.222	24.731	-10.385	1.00	12.70
ATOM	3163	N	SER	B	43	19.633	23.642	-9.935	1.00	13.40
ATOM	3164	CA	SER	B	43	18.551	25.613	-9.641	1.00	10.83
ATOM	3165	CB	SER	B	43	18.212	25.317	-8.240	1.00	13.03

Figure 1 (continued 32)

ATOM	3166	CB	SER	B	43	18.605	26.457	-7.298	1.00	15.48	B
ATOM	3167	OG	SER	B	43	20.017	26.635	-7.258	1.00	16.36	B
ATOM	3168	CO	SER	B	43	16.699	25.141	-8.194	1.00	12.37	B
ATOM	3169	CO	SER	B	43	15.953	25.873	-8.875	1.00	13.81	B
ATOM	3170	N	LEU	B	44	16.259	24.133	-7.427	1.00	12.48	B
ATOM	3171	CA	LEU	B	44	14.832	23.840	-7.249	1.00	11.34	B
ATOM	3172	CB	LEU	B	44	14.504	22.413	-7.724	1.00	12.56	B
ATOM	3173	CG	LEU	B	44	14.993	22.028	-9.122	1.00	14.70	B
ATOM	3174	CD1	LEU	B	44	14.964	20.500	-9.306	1.00	18.40	B
ATOM	3175	CD2	LEU	B	44	14.105	22.717	-10.133	1.00	19.25	B
ATOM	3176	C	LEU	B	44	14.581	23.918	-5.746	1.00	13.84	B
ATOM	3177	O	LEU	B	44	15.344	23.356	-4.936	1.00	12.96	B
ATOM	3178	N	THR	B	45	13.499	24.583	-5.359	1.00	11.87	B
ATOM	3179	CA	THR	B	45	13.179	24.726	-3.928	1.00	13.31	B
ATOM	3180	CB	THR	B	45	13.481	26.166	-3.421	1.00	13.75	B
ATOM	3181	OG1	THR	B	45	14.869	26.485	-3.627	1.00	15.13	B
ATOM	3182	CG2	THR	B	45	13.157	26.269	-1.922	1.00	14.06	B
ATOM	3183	CG	THR	B	45	11.698	24.477	-3.666	1.00	14.00	B
ATOM	3184	CO	THR	B	45	10.867	24.948	-4.423	1.00	13.55	B
ATOM	3185	N	GLY	B	46	11.396	23.696	-2.631	1.00	13.36	B
ATOM	3186	CA	GLY	B	46	10.029	23.408	-2.203	1.00	13.22	B
ATOM	3187	N	GLY	B	46	9.898	23.843	-0.738	1.00	14.39	B
ATOM	3188	CO	GLY	B	46	10.856	23.711	0.017	1.00	15.56	B
ATOM	3189	N	THR	B	47	8.736	24.387	-0.333	1.00	14.57	B
ATOM	3190	CA	THR	B	47	8.592	24.822	1.061	1.00	15.34	B
ATOM	3191	CB	THR	B	47	8.985	26.317	1.236	1.00	16.19	B
ATOM	3192	OG1	THR	B	47	9.049	26.655	2.632	1.00	15.79	B
ATOM	3193	CG2	THR	B	47	7.967	27.253	0.564	1.00	17.31	B
ATOM	3194	C	THR	B	47	7.162	24.668	1.564	1.00	16.59	B
ATOM	3195	CO	THR	B	47	6.226	24.562	0.768	1.00	16.42	B
ATOM	3196	N	ASP	B	48	7.009	24.615	2.887	1.00	17.13	B
ATOM	3197	CA	ASP	B	48	5.658	24.598	3.487	1.00	16.11	B
ATOM	3198	CB	ASP	B	48	5.344	23.244	4.132	1.00	15.80	B
ATOM	3199	CG	ASP	B	48	6.136	22.986	5.398	1.00	16.28	B
ATOM	3200	OD1	ASP	B	48	7.041	23.773	5.722	1.00	16.79	B
ATOM	3201	OD2	ASP	B	48	5.825	21.976	6.074	1.00	20.58	B
ATOM	3202	C	ASP	B	48	5.559	25.736	4.521	1.00	18.07	B
ATOM	3203	O	ASP	B	48	4.612	25.768	5.321	1.00	18.39	B
ATOM	3204	N	LEU	B	49	6.545	26.641	4.479	1.00	15.86	B
ATOM	3205	CA	LEU	B	49	6.712	27.827	5.343	1.00	17.77	B
ATOM	3206	CB	LEU	B	49	5.383	28.520	5.666	1.00	17.51	B
ATOM	3207	CG	LEU	B	49	4.676	29.110	4.453	1.00	17.64	B
ATOM	3208	CD1	LEU	B	49	3.373	29.816	4.956	1.00	21.50	B
ATOM	3209	CD2	LEU	B	49	5.594	30.102	3.756	1.00	19.20	B
ATOM	3210	C	LEU	B	49	7.406	27.475	6.656	1.00	16.84	B
ATOM	3211	O	LEU	B	49	7.860	28.372	7.370	1.00	20.06	B
ATOM	3212	N	GLU	B	50	7.467	26.189	6.991	1.00	17.57	B
ATOM	3213	CA	GLU	B	50	8.164	25.802	8.228	1.00	16.55	B
ATOM	3214	CB	GLU	B	50	7.359	24.747	9.000	1.00	20.80	B
ATOM	3215	CG	GLU	B	50	7.969	24.377	10.373	1.00	25.34	B
ATOM	3216	CD	GLU	B	50	7.109	23.396	11.186	1.00	29.02	B
ATOM	3217	OE1	GLU	B	50	7.079	23.504	12.435	1.00	30.09	B
ATOM	3218	OE2	GLU	B	50	6.487	22.496	10.592	1.00	31.29	B
ATOM	3219	C	GLU	B	50	9.540	25.238	7.842	1.00	16.32	B
ATOM	3220	O	GLU	B	50	10.511	25.373	8.580	1.00	16.99	B
ATOM	3221	N	MET	B	51	9.611	24.630	6.672	1.00	15.47	B
ATOM	3222	CA	MET	B	51	10.882	24.074	6.215	1.00	14.90	B
ATOM	3223	CB	MET	B	51	10.987	22.609	6.653	1.00	15.67	B
ATOM	3224	CG	MET	B	51	9.910	21.720	6.114	1.00	17.25	B
ATOM	3225	SD	MET	B	51	9.719	20.228	7.113	1.00	21.05	B
ATOM	3226	CE	MET	B	51	8.965	20.945	8.604	1.00	23.10	B
ATOM	3227	C	MET	B	51	10.988	24.187	4.721	1.00	14.86	B
ATOM	3228	O	MET	B	51	9.978	24.437	4.029	1.00	15.26	B
ATOM	3229	N	GLU	B	52	12.210	24.027	4.202	1.00	14.83	B
ATOM	3230	CA	GLU	B	52	12.367	24.087	2.755	1.00	13.34	B
ATOM	3231	CB	GLU	B	52	12.761	25.477	2.295	1.00	18.93	B
ATOM	3232	CG	GLU	B	52	13.998	26.005	2.925	1.00	25.39	B
ATOM	3233	CD	GLU	B	52	14.361	27.374	2.411	1.00	31.84	B
ATOM	3234	OE1	GLU	B	52	13.504	28.295	2.473	1.00	32.96	B
ATOM	3235	OE2	GLU	B	52	15.520	27.508	1.960	1.00	35.26	B
ATOM	3236	C	GLU	B	52	13.420	23.100	2.339	1.00	14.63	B
ATOM	3237	O	GLU	B	52	14.317	22.798	3.108	1.00	13.33	B
ATOM	3238	N	MET	B	53	13.314	22.604	1.117	1.00	14.02	B
ATOM	3239	CA	MET	B	53	14.280	21.636	0.610	1.00	16.35	B
ATOM	3240	CB	MET	B	53	13.675	20.289	0.379	1.00	19.16	B
ATOM	3241	CG	MET	B	53	14.496	19.209	-0.220	1.00	23.65	B
ATOM	3242	SD	MET	B	53	15.833	18.696	0.914	1.00	20.87	B
ATOM	3243	CE	MET	B	53	14.878	17.649	1.951	1.00	14.06	B
ATOM	3244	C	MET	B	53	14.777	22.225	-0.701	1.00	13.90	B
ATOM	3245	O	MET	B	53	13.977	22.607	-1.546	1.00	13.10	B
ATOM	3246	N	VAL	B	54	16.091	22.294	-0.872	1.00	13.22	B
ATOM	3247	CA	VAL	B	54	16.687	22.882	-2.089	1.00	14.45	B
ATOM	3248	CB	VAL	B	54	17.539	24.079	-1.725	1.00	14.52	B
ATOM	3249	CG1	VAL	B	54	18.117	24.704	-2.984	1.00	13.15	B
ATOM	3250	CG2	VAL	B	54	16.699	25.088	-0.938	1.00	13.82	B
ATOM	3251	C	VAL	B	54	17.590	21.867	-2.768	1.00	16.01	B
ATOM	3252	O	VAL	B	54	18.330	21.169	-2.093	1.00	11.25	B
ATOM	3253	N	ALA	B	55	17.513	21.765	-4.096	1.00	13.21	B
ATOM	3254	CA	ALA	B	55	18.380	20.865	-4.850	1.00	12.81	B
ATOM	3255	CB	ALA	B	55	17.548	19.820	-5.605	1.00	15.53	B
ATOM	3256	C	ALA	B	55	19.144	21.706	-5.863	1.00	15.73	B
ATOM	3257	O	ALA	B	55	18.564	22.606	-6.461	1.00	14.23	B
ATOM	3258	N	ARG	B	56	20.433	21.410	-6.059	1.00	15.31	B
ATOM	3259	CA	ARG	B	56	21.258	22.119	-7.044	1.00	16.38	B
ATOM	3260	CB	ARG	B	56	22.601	22.523	-6.432	1.00	22.20	B
ATOM	3261	CG	ARG	B	56	22.482	23.229	-5.112	1.00	24.40	B
ATOM	3262	CD	ARG	B	56	22.101	24.643	-5.283	1.00	26.52	B
ATOM	3263	NE	ARG	B	56	22.131	25.327	-3.990	1.00	27.62	B
ATOM	3264	CZ	ARG	B	56	21.494	26.463	-3.729	1.00	23.46	B
ATOM	3265	NH1	ARG	B	56	20.779	27.069	-4.676	1.00		B

Figure 1 (continued 33)

[illegible][illegible]

ATOM	3366	C	VAL	B	70	4.913	25.183	-10.490	1.00	12.72
ATOM	3367	O	VAL	B	70	5.550	24.803	-9.489	1.00	12.07
ATOM	3368	N	PRO	B	71	3.734	24.651	-10.825	1.00	12.89
ATOM	3369	C	PRO	B	71	2.872	25.050	-11.964	1.00	14.31
ATOM	3370	CA	PRO	B	71	3.129	23.572	-10.016	1.00	12.87
ATOM	3371	CB	PRO	B	71	1.845	23.239	-10.756	1.00	14.80
ATOM	3372	CG	PRO	B	71	1.522	24.614	-11.481	1.00	19.52
ATOM	3373	C	PRO	B	71	4.044	22.363	-9.848	1.00	12.82
ATOM	3374	O	ALA	B	72	4.480	21.743	-10.813	1.00	13.40
ATOM	3375	N	ALA	B	72	4.340	22.035	-8.599	1.00	11.96
ATOM	3376	CA	ALA	B	72	5.293	20.944	-8.344	1.00	12.77
ATOM	3377	CB	ALA	B	72	5.611	20.907	-6.847	1.00	13.14
ATOM	3378	C	ALA	B	72	4.857	19.587	-8.805	1.00	11.71
ATOM	3379	O	ARG	B	73	5.618	18.899	-9.515	1.00	12.89
ATOM	3380	N	ARG	B	73	3.654	19.178	-8.426	1.00	15.37
ATOM	3381	CA	ARG	B	73	3.155	17.856	-8.777	1.00	19.29
ATOM	3382	CB	ARG	B	73	1.769	17.634	-8.137	1.00	28.52
ATOM	3383	CG	ARG	B	73	1.189	16.241	-8.362	1.00	33.56
ATOM	3384	CD	ARG	B	73	2.091	15.198	-7.713	1.00	39.25
ATOM	3385	NE	ARG	B	73	1.915	13.882	-8.310	1.00	39.95
ATOM	3386	CZ	ARG	B	73	2.786	12.882	-8.182	1.00	40.90
ATOM	3387	NH1	ARG	B	73	3.894	13.052	-7.476	1.00	41.65
ATOM	3388	NH2	ARG	B	73	2.549	11.711	-8.772	1.00	12.85
ATOM	3389	C	ARG	B	73	3.074	17.695	-10.292	1.00	12.28
ATOM	3390	O	LYS	B	74	3.480	16.668	-10.851	1.00	12.56
ATOM	3391	N	LYS	B	74	2.530	18.708	-10.956	1.00	12.58
ATOM	3392	CA	LYS	B	74	2.387	18.655	-12.419	1.00	11.93
ATOM	3393	CB	LYS	B	74	1.647	19.886	-12.933	1.00	13.85
ATOM	3394	CG	LYS	B	74	0.149	19.815	-12.596	1.00	15.33
ATOM	3395	CD	LYS	B	74	-0.493	21.183	-12.811	1.00	16.90
ATOM	3396	CE	LYS	B	74	-1.982	21.112	-12.597	1.00	17.31
ATOM	3397	NZ	LYS	B	74	-2.482	22.535	-12.538	1.00	11.10
ATOM	3398	C	LYS	B	74	3.729	18.561	-13.101	1.00	11.83
ATOM	3399	O	PHE	B	75	3.882	17.738	-14.009	1.00	11.16
ATOM	3400	N	PHE	B	75	4.687	19.379	-12.673	1.00	8.77
ATOM	3401	CA	PHE	B	75	6.015	19.357	-13.326	1.00	9.59
ATOM	3402	CB	PHE	B	75	6.851	20.553	-12.866	1.00	11.61
ATOM	3403	CG	PHE	B	75	8.199	20.686	-13.568	1.00	12.29
ATOM	3404	CD1	PHE	B	75	8.300	20.587	-14.956	1.00	12.93
ATOM	3405	CD2	PHE	B	75	9.320	20.975	-12.835	1.00	14.18
ATOM	3406	CE1	PHE	B	75	9.567	20.782	-15.596	1.00	16.28
ATOM	3407	CE2	PHE	B	75	10.561	21.172	-13.448	1.00	13.85
ATOM	3408	CZ	PHE	B	75	10.677	21.069	-14.836	1.00	10.84
ATOM	3409	C	PHE	B	75	6.699	18.029	-13.066	1.00	9.16
ATOM	3410	O	PHE	B	75	7.225	17.420	-14.009	1.00	10.39
ATOM	3411	N	PHE	B	76	6.663	17.552	-11.819	1.00	11.16
ATOM	3412	CA	PHE	B	76	7.252	16.230	-11.555	1.00	12.22
ATOM	3413	CB	PHE	B	76	7.138	15.862	-10.092	1.00	14.40
ATOM	3414	CG	PHE	B	76	7.546	14.459	-9.823	1.00	16.66
ATOM	3415	CD1	PHE	B	76	8.888	14.117	-9.730	1.00	17.02
ATOM	3416	CD2	PHE	B	76	6.583	13.475	-9.667	1.00	17.99
ATOM	3417	CE1	PHE	B	76	9.252	12.795	-9.461	1.00	18.48
ATOM	3418	CE2	PHE	B	76	6.946	12.143	-9.407	1.00	12.82
ATOM	3419	CZ	PHE	B	76	8.275	11.821	-9.302	1.00	10.50
ATOM	3420	C	PHE	B	76	6.579	15.133	-12.373	1.00	10.55
ATOM	3421	O	ASP	B	77	5.247	14.307	-12.999	1.00	9.78
ATOM	3422	N	ASP	B	77	4.563	15.103	-12.399	1.00	17.39
ATOM	3423	CA	ASP	B	77	3.053	14.074	-13.173	1.00	17.35
ATOM	3424	CB	ASP	B	77	2.626	14.178	-12.970	1.00	18.13
ATOM	3425	CG	ASP	B	77	3.429	13.732	-11.596	1.00	8.50
ATOM	3426	OD1	ASP	B	77	1.441	13.121	-10.843	1.00	10.06
ATOM	3427	OD2	ASP	B	77	4.893	14.113	-11.260	1.00	9.33
ATOM	3428	C	ASP	B	77	5.004	13.055	-14.663	1.00	9.86
ATOM	3429	O	ASP	B	77	5.065	15.316	-15.288	1.00	11.48
ATOM	3430	N	ILE	B	78	5.427	15.449	-15.218	1.00	13.90
ATOM	3431	CA	ILE	B	78	5.451	16.940	-17.049	1.00	13.19
ATOM	3432	CB	ILE	B	78	6.191	17.139	-18.424	1.00	16.24
ATOM	3433	CG1	ILE	B	78	3.976	17.389	-17.151	1.00	9.23
ATOM	3434	CG2	ILE	B	78	3.776	18.939	-17.260	1.00	10.91
ATOM	3435	CD1	ILE	B	78	6.817	14.832	-16.839	1.00	10.15
ATOM	3436	C	ILE	B	78	6.993	13.993	-17.726	1.00	10.57
ATOM	3437	O	CYS	B	79	7.762	15.226	-16.013	1.00	10.45
ATOM	3438	N	CYS	B	79	9.131	14.699	-16.223	1.00	15.50
ATOM	3439	CA	CYS	B	79	10.081	15.403	-15.269	1.00	12.39
ATOM	3440	CB	CYS	B	79	10.273	17.176	-15.649	1.00	13.55
ATOM	3441	CG	CYS	B	79	9.176	13.190	-16.024	1.00	10.64
ATOM	3442	O	ARG	B	80	9.819	12.455	-16.788	1.00	12.98
ATOM	3443	N	ARG	B	80	8.500	12.725	-14.986	1.00	15.52
ATOM	3444	CA	ARG	B	80	8.491	11.273	-14.719	1.00	20.13
ATOM	3445	CB	ARG	B	80	7.744	11.007	-13.399	1.00	25.38
ATOM	3446	CG	ARG	B	80	7.791	9.534	-12.911	1.00	31.58
ATOM	3447	CD	ARG	B	80	6.843	9.325	-11.713	1.00	33.35
ATOM	3448	NE	ARG	B	80	5.482	9.714	-12.093	1.00	35.49
ATOM	3449	CZ	ARG	B	80	4.456	9.888	-11.254	1.00	34.33
ATOM	3450	NH1	ARG	B	80	4.598	9.704	-9.939	1.00	13.18
ATOM	3451	NH2	ARG	B	80	3.280	10.257	-11.732	1.00	13.55
ATOM	3452	C	ARG	B	80	7.819	10.507	-15.846	1.00	11.84
ATOM	3453	O	ARG	B	80	8.159	9.360	-16.140	1.00	11.90
ATOM	3454	N	GLY	B	81	6.836	11.128	-16.484	1.00	11.01
ATOM	3455	CA	GLY	B	81	6.116	10.437	-17.522	1.00	11.50
ATOM	3456	C	GLY	B	81	6.781	10.356	-18.869	1.00	11.31
ATOM	3457	O	GLY	B	81	6.335	9.605	-19.734	1.00	9.84
ATOM	3458	N	LEU	B	82	7.806	11.188	-19.071	1.00	8.66
ATOM	3459	CA	LEU	B	82	8.514	11.169	-20.328	1.00	9.38
ATOM	3460	CB	LEU	B	82	9.370	12.430	-20.446	1.00	9.37
ATOM	3461	CG	LEU	B	82	8.522	13.680	-20.801	1.00	11.14
ATOM	3462	CD1	LEU	B	82	9.372	14.967	-20.574	1.00	11.17
ATOM	3463	CD2	LEU	B	82	8.050	13.551	-22.262	1.00	
ATOM	3464	C	LEU	B	82	9.376	9.916	-20.380	1.00	

Figure 1 (continued 35)

ATOM	3466	O	LEU	B	82	9.726	9.344	-19.347	1.00	12.58	B
ATOM	3467	N	PRO	B	83	9.758	9.523	-21.590	1.00	11.69	B
ATOM	3468	CD	PRO	B	83	9.531	10.208	-22.863	1.00	13.36	B
ATOM	3469	CA	PRO	B	83	10.575	8.309	-21.770	1.00	12.94	B
ATOM	3470	CB	PRO	B	83	10.597	8.140	-23.290	1.00	15.08	B
ATOM	3471	CG	PRO	B	83	10.505	9.493	-23.806	1.00	14.86	B
ATOM	3472	C	PRO	B	83	11.964	8.393	-21.150	1.00	15.17	B
ATOM	3473	O	PRO	B	83	12.542	9.473	-21.023	1.00	14.86	B
ATOM	3474	N	GLU	B	84	12.495	7.237	-20.759	1.00	15.45	B
ATOM	3475	CA	GLU	B	84	13.817	7.220	-20.152	1.00	15.30	B
ATOM	3476	CB	GLU	B	84	14.193	5.761	-19.825	1.00	17.19	B
ATOM	3477	CG	GLU	B	84	15.507	5.588	-19.128	1.00	20.25	B
ATOM	3478	CD	GLU	B	84	15.564	4.266	-18.419	1.00	22.78	B
ATOM	3479	OE1	GLU	B	84	14.981	3.297	-18.955	1.00	27.86	B
ATOM	3480	OE2	GLU	B	84	16.180	4.197	-17.344	1.00	25.77	B
ATOM	3481	C	GLU	B	84	14.831	7.848	-21.116	1.00	13.55	B
ATOM	3482	O	GLU	B	84	14.815	7.576	-22.325	1.00	16.08	B
ATOM	3483	N	GLY	B	85	15.682	8.719	-20.573	1.00	15.12	B
ATOM	3484	CA	GLY	B	85	16.714	9.359	-21.386	1.00	15.70	B
ATOM	3485	C	GLY	B	85	16.279	10.612	-22.136	1.00	16.21	B
ATOM	3486	O	GLY	B	85	17.088	11.268	-22.797	1.00	17.94	B
ATOM	3487	N	ALA	B	86	14.995	10.955	-22.013	1.00	13.60	B
ATOM	3488	CA	ALA	B	86	14.450	12.128	-22.688	1.00	13.37	B
ATOM	3489	CB	ALA	B	86	12.944	12.293	-22.330	1.00	15.70	B
ATOM	3490	C	ALA	B	86	15.161	13.416	-22.324	1.00	12.98	B
ATOM	3491	O	ALA	B	86	15.551	13.631	-21.183	1.00	12.60	B
ATOM	3492	N	GLU	B	87	15.341	14.285	-23.316	1.00	12.20	B
ATOM	3493	CA	GLU	B	87	15.926	15.594	-23.086	1.00	16.46	B
ATOM	3494	CB	GLU	B	87	16.650	16.050	-24.339	1.00	20.50	B
ATOM	3495	CG	GLU	B	87	17.818	15.137	-24.688	1.00	24.25	B
ATOM	3496	CD	GLU	B	87	18.945	15.208	-23.669	1.00	21.60	B
ATOM	3497	OE1	GLU	B	87	18.958	16.145	-22.844	1.00	25.73	B
ATOM	3498	OE2	GLU	B	87	19.827	14.308	-23.718	1.00	12.64	B
ATOM	3499	C	GLU	B	87	14.734	16.512	-22.814	1.00	15.78	B
ATOM	3500	O	GLU	B	87	13.810	16.527	-23.623	1.00	12.08	B
ATOM	3501	N	ILE	B	88	14.770	17.241	-21.707	1.00	11.17	B
ATOM	3502	CA	ILE	B	88	13.645	18.127	-21.325	1.00	11.48	B
ATOM	3503	CB	ILE	B	88	13.218	17.788	-19.878	1.00	12.56	B
ATOM	3504	CG2	ILE	B	88	11.990	18.637	-19.452	1.00	12.51	B
ATOM	3505	CG1	ILE	B	88	12.887	16.294	-19.815	1.00	11.91	B
ATOM	3506	CD1	ILE	B	88	12.482	15.794	-18.471	1.00	10.83	B
ATOM	3507	C	ILE	B	88	14.067	19.573	-21.468	1.00	12.26	B
ATOM	3508	O	ILE	B	88	14.909	20.066	-20.691	1.00	10.23	B
ATOM	3509	N	ALA	B	89	13.477	20.261	-22.448	1.00	11.36	B
ATOM	3510	CA	ALA	B	89	13.802	21.659	-22.723	1.00	11.07	B
ATOM	3511	CB	ALA	B	89	13.784	21.911	-24.227	1.00	12.01	B
ATOM	3512	O	ALA	B	89	12.738	22.517	-22.046	1.00	10.02	B
ATOM	3513	N	VAL	B	90	11.542	22.297	-22.226	1.00	9.76	B
ATOM	3514	CA	VAL	B	90	13.196	23.508	-21.307	1.00	10.85	B
ATOM	3515	CB	VAL	B	90	12.301	24.367	-20.549	1.00	12.19	B
ATOM	3516	CG1	VAL	B	90	12.499	24.064	-19.045	1.00	11.27	B
ATOM	3517	CG2	VAL	B	90	11.583	24.955	-18.217	1.00	11.53	B
ATOM	3518	C	VAL	B	90	12.171	22.613	-18.750	1.00	13.48	B
ATOM	3519	O	VAL	B	90	12.577	25.830	-20.791	1.00	11.55	B
ATOM	3520	N	GLN	B	91	13.731	26.256	-20.768	1.00	14.62	B
ATOM	3521	CA	GLN	B	91	11.523	26.617	-21.015	1.00	18.48	B
ATOM	3522	CB	GLN	B	91	11.705	28.051	-21.210	1.00	26.33	B
ATOM	3523	CG	GLN	B	91	11.889	28.401	-22.692	1.00	29.12	B
ATOM	3524	CD	GLN	B	91	12.135	29.913	-22.891	1.00	34.56	B
ATOM	3525	OE1	GLN	B	91	12.980	30.211	-24.112	1.00	31.87	B
ATOM	3526	OE2	GLN	B	91	13.538	31.308	-24.238	1.00	14.08	B
ATOM	3527	NE2	GLN	B	91	13.073	29.248	-25.024	1.00	13.76	B
ATOM	3528	C	GLN	B	91	10.550	28.838	-20.631	1.00	14.73	B
ATOM	3529	O	GLN	B	91	9.367	28.487	-20.811	1.00	15.30	B
ATOM	3530	N	LEU	B	92	10.908	29.885	-19.884	1.00	16.00	B
ATOM	3531	CA	LEU	B	92	9.928	30.771	-19.267	1.00	15.51	B
ATOM	3532	CB	LEU	B	92	10.575	31.606	-18.144	1.00	18.05	B
ATOM	3533	CG	LEU	B	92	9.626	32.613	-17.459	1.00	17.67	B
ATOM	3534	CD1	LEU	B	92	8.460	31.882	-16.765	1.00	16.50	B
ATOM	3535	CD2	LEU	B	92	10.387	33.405	-16.426	1.00	17.36	B
ATOM	3536	C	LEU	B	92	9.435	31.694	-20.368	1.00	17.70	B
ATOM	3537	O	LEU	B	92	10.259	32.293	-21.102	1.00	20.10	B
ATOM	3538	N	GLU	B	93	8.107	31.790	-20.487	1.00	19.07	B
ATOM	3539	CA	GLU	B	93	7.456	32.645	-21.469	1.00	20.16	B
ATOM	3540	CB	GLU	B	93	6.889	31.788	-22.615	1.00	21.44	B
ATOM	3541	CG	GLU	B	93	8.021	30.998	-23.341	1.00	22.08	B
ATOM	3542	CD	GLU	B	93	7.622	30.371	-24.678	1.00	20.59	B
ATOM	3543	OE1	GLU	B	93	6.413	30.147	-24.893	1.00	21.41	B
ATOM	3544	OE2	GLU	B	93	8.530	30.087	-25.504	1.00	22.54	B
ATOM	3545	C	GLU	B	93	6.358	33.451	-20.767	1.00	23.49	B
ATOM	3546	O	GLU	B	93	5.165	33.286	-21.039	1.00	23.13	B
ATOM	3547	N	GLY	B	94	6.774	34.296	-19.821	1.00	23.80	B
ATOM	3548	CA	GLY	B	94	5.826	35.136	-19.099	1.00	23.56	B
ATOM	3549	C	GLY	B	94	4.835	34.435	-18.182	1.00	21.90	B
ATOM	3550	O	GLY	B	94	5.205	33.923	-17.126	1.00	22.03	B
ATOM	3551	N	GLU	B	95	3.569	34.428	-18.574	1.00	25.70	B
ATOM	3552	CA	GLU	B	95	2.539	33.797	-17.756	1.00	32.06	B
ATOM	3553	CB	GLU	B	95	1.135	34.201	-18.269	1.00	34.90	B
ATOM	3554	CG	GLU	B	95	0.715	33.489	-19.565	1.00	35.44	B
ATOM	3555	CD	GLU	B	95	-0.577	34.015	-20.188	1.00	37.09	B
ATOM	3556	OE1	GLU	B	95	-1.491	34.428	-19.437	1.00	20.12	B
ATOM	3557	OE2	GLU	B	95	-0.679	33.994	-21.442	1.00	19.55	B
ATOM	3558	C	GLU	B	95	2.680	32.262	-17.760	1.00	17.37	B
ATOM	3559	O	GLU	B	95	2.076	31.573	-16.932	1.00	14.55	B
ATOM	3560	N	ARG	B	96	3.465	31.726	-18.694	1.00	16.86	B
ATOM	3561	CA	ARG	B	96	3.605	30.271	-18.751	1.00	16.89	B
ATOM	3562	CB	ARG	B	96	2.777	29.683	-19.912	1.00	20.34	B
ATOM	3563	CG	ARG	B	96	3.296	29.992	-21.341	1.00	22.54	B
ATOM	3564	CD	ARG	B	96	4.258	28.903	-21.876	1.00		B
ATOM	3565	NE	ARG	B	96	4.551	28.994	-23.319	1.00		B

Figure 1 (continued 36)

ATOM	3566	CZ	ARG	B	96	3.842	28.445	-24.308	1.00	25.11
ATOM	3567	NH1	ARG	B	96	2.742	27.746	-24.054	1.00	24.38
ATOM	3568	NH2	ARG	B	96	4.276	28.546	-25.577	1.00	20.68
ATOM	3569	C	ARG	B	96	5.025	29.829	-18.904	1.00	13.94
ATOM	3570	O	MET	B	97	5.883	30.602	-19.331	1.00	14.85
ATOM	3571	N	MET	B	97	5.266	28.578	-18.520	1.00	12.30
ATOM	3572	CA	MET	B	97	6.582	27.961	-17.326	1.00	10.91
ATOM	3573	CB	MET	B	97	7.093	27.392	-17.487	1.00	10.86
ATOM	3574	CG	MET	B	97	8.503	26.885	-15.952	1.00	14.36
ATOM	3575	SD	MET	B	97	9.268	26.288	-15.920	1.00	14.09
ATOM	3576	CE	MET	B	97	8.674	24.617	-19.641	1.00	11.29
ATOM	3577	C	MET	B	97	6.336	26.817	-19.386	1.00	11.55
ATOM	3578	O	LEU	B	98	5.493	25.956	-20.750	1.00	10.37
ATOM	3579	N	LEU	B	98	7.099	26.798	-21.793	1.00	9.09
ATOM	3580	CA	LEU	B	98	6.935	25.818	-23.145	1.00	10.04
ATOM	3581	CB	LEU	B	98	7.140	26.502	-24.343	1.00	13.03
ATOM	3582	CG	LEU	B	98	7.119	25.556	-24.484	1.00	14.58
ATOM	3583	CD1	LEU	B	98	5.756	24.875	-25.593	1.00	15.51
ATOM	3584	CD2	LEU	B	98	7.499	26.390	-21.615	1.00	10.17
ATOM	3585	C	LEU	B	98	7.936	24.703	-21.439	1.00	12.00
ATOM	3586	N	VAL	B	99	9.121	24.991	-21.569	1.00	8.14
ATOM	3587	CA	VAL	B	99	7.440	23.469	-20.182	1.00	9.99
ATOM	3588	CB	VAL	B	99	8.303	22.284	-18.916	1.00	12.22
ATOM	3589	CG1	VAL	B	99	7.831	21.408	-22.700	1.00	11.04
ATOM	3590	CG2	VAL	B	99	8.712	20.156	-23.108	1.00	10.88
ATOM	3591	C	VAL	B	99	7.813	22.225	-24.593	1.00	8.30
ATOM	3592	O	VAL	B	99	8.169	21.454	-25.829	1.00	10.50
ATOM	3593	N	ARG	B	100	7.031	21.087	-26.057	1.00	11.28
ATOM	3594	CA	ARG	B	100	9.293	21.137	-27.152	1.00	15.41
ATOM	3595	CB	ARG	B	100	9.218	20.368	-27.375	1.00	16.70
ATOM	3596	CG	ARG	B	100	9.613	21.220	-28.526	1.00	17.28
ATOM	3597	CD	ARG	B	100	8.754	22.464	-26.876	1.00	21.89
ATOM	3598	NE	ARG	B	100	9.404	23.363	-24.523	1.00	22.39
ATOM	3599	NH1	ARG	B	100	10.676	23.920	-25.051	1.00	9.77
ATOM	3600	NH2	ARG	B	100	11.829	23.803	-25.125	1.00	7.91
ATOM	3601	C	ARG	B	100	11.889	23.144	-23.787	1.00	10.45
ATOM	3602	O	ARG	B	100	12.927	24.341	-23.840	1.00	13.17
ATOM	3603	N	SER	B	101	10.176	19.198	-26.265	1.00	12.22
ATOM	3604	CA	SER	B	101	11.283	19.325	-27.235	1.00	11.21
ATOM	3605	CB	SER	B	101	9.725	18.074	-28.376	1.00	11.77
ATOM	3606	CG	SER	B	101	10.578	16.881	-29.010	1.00	11.95
ATOM	3607	C	SER	B	101	10.549	16.126	-29.277	1.00	13.86
ATOM	3608	O	SER	B	101	11.462	14.998	-29.248	1.00	13.24
ATOM	3609	N	GLY	B	102	10.043	16.057	-31.024	1.00	15.71
ATOM	3610	CA	GLY	B	102	8.875	15.686	-33.491	1.00	20.42
ATOM	3611	CB	GLY	B	102	10.900	15.720	-33.518	1.00	21.82
ATOM	3612	CG	GLY	B	102	10.396	14.967	-34.539	1.00	24.65
ATOM	3613	O	ARG	B	103	9.269	15.772	-34.517	1.00	25.63
ATOM	3614	N	ARG	B	103	9.440	16.944	-28.966	1.00	13.10
ATOM	3615	CA	ARG	B	103	8.113	15.137	-27.468	1.00	14.85
ATOM	3616	CB	ARG	B	103	6.950	15.842	-26.293	1.00	10.09
ATOM	3617	CG	ARG	B	103	6.404	15.140	-25.138	1.00	11.86
ATOM	3618	CD	ARG	B	103	7.403	15.240	-25.597	1.00	12.18
ATOM	3619	NE	ARG	B	103	6.753	14.857	-25.877	1.00	12.05
ATOM	3620	CZ	ARG	B	103	6.426	13.446	-25.815	1.00	12.30
ATOM	3621	NH1	ARG	B	103	5.798	12.861	-25.625	1.00	10.81
ATOM	3622	NH2	ARG	B	103	5.437	13.580	-26.370	1.00	10.24
ATOM	3623	C	ARG	B	103	5.564	11.560	-27.618	1.00	12.01
ATOM	3624	O	ARG	B	103	5.893	15.933	-28.760	1.00	12.34
ATOM	3625	N	SER	B	104	4.685	15.809	-28.364	1.00	13.57
ATOM	3626	CA	SER	B	104	6.372	16.100	-28.366	1.00	13.32
ATOM	3627	CB	SER	B	104	5.503	16.309	-28.740	1.00	14.90
ATOM	3628	CG	SER	B	104	5.888	15.378	-28.014	1.00	13.50
ATOM	3629	CD	SER	B	104	5.938	14.020	-24.052	1.00	14.92
ATOM	3630	C	SER	B	104	5.701	17.775	-24.006	1.00	9.77
ATOM	3631	O	ARG	B	105	6.849	18.298	-23.108	1.00	11.33
ATOM	3632	N	ARG	B	105	4.587	18.470	-21.939	1.00	10.77
ATOM	3633	CA	ARG	B	105	4.659	19.867	-20.719	1.00	9.20
ATOM	3634	CB	ARG	B	105	4.158	20.772	-21.000	1.00	10.28
ATOM	3635	CG	ARG	B	105	5.004	20.772	-21.591	1.00	12.41
ATOM	3636	CD	ARG	B	105	4.285	21.560	-20.793	1.00	12.06
ATOM	3637	NE	ARG	B	105	3.799	22.896	-21.982	1.00	12.35
ATOM	3638	CZ	ARG	B	105	4.552	23.991	-21.182	1.00	13.89
ATOM	3639	NH1	ARG	B	105	5.822	23.903	-21.783	1.00	14.71
ATOM	3640	NH2	ARG	B	105	4.037	25.165	-21.579	1.00	12.00
ATOM	3641	C	ARG	B	105	3.757	20.122	-21.528	1.00	11.63
ATOM	3642	O	PHE	B	106	2.639	19.588	-21.291	1.00	10.03
ATOM	3643	N	PHE	B	106	4.221	20.929	-20.896	1.00	13.00
ATOM	3644	CA	PHE	B	106	3.380	21.252	-21.848	1.00	13.92
ATOM	3645	CB	PHE	B	106	3.795	20.410	-21.475	1.00	17.21
ATOM	3646	CG	PHE	B	106	3.876	18.955	-19.471	1.00	13.30
ATOM	3647	CD1	PHE	B	106	5.019	18.433	-18.219	1.00	13.25
ATOM	3648	CD2	PHE	B	106	2.775	18.115	-17.130	1.00	11.97
ATOM	3649	CE1	PHE	B	106	5.072	17.120	-16.221	1.00	12.30
ATOM	3650	CE2	PHE	B	106	2.812	16.797	-15.427	1.00	13.26
ATOM	3651	CZ	PHE	B	106	3.953	16.280	-15.567	1.00	15.24
ATOM	3652	O	PHE	B	106	3.525	22.714	-16.079	1.00	14.96
ATOM	3653	N	SER	B	107	4.649	23.241		1.00	15.65
ATOM	3654	CA	SER	B	107	2.389	23.375			
ATOM	3655	CB	SER	B	107	2.415	24.766			
ATOM	3656	CG	SER	B	107	1.559	25.595			
ATOM	3657	CD	SER	B	107	1.547	26.962			
ATOM	3658	O	SER	B	107	1.897	24.858			
ATOM	3659	N	LEU	B	108	0.741	24.542			
ATOM	3660	CA	LEU	B	108	2.774	25.213			
ATOM	3661	CB	LEU	B	108	2.399	25.325			
ATOM	3662	CG	LEU	B	108	3.497	24.741			
ATOM	3663	CD1	LEU	B	108	3.715	23.249			
ATOM	3664	CD2	LEU	B	108	4.883	22.751			
ATOM	3665					2.441	22.561			

Figure 1 (continued 37)

ATOM	3666	C	LEU	B	108	2.210	26.768	-16.703	1.00	12.13	
ATOM	3667	O	LEU	B	108	2.936	27.647	-17.149	1.00	12.73	
ATOM	3668	N	SER	B	109	1.249	27.021	-15.807	1.00	13.50	
ATOM	3669	CA	SER	B	109	1.036	28.382	-15.313	1.00	15.61	
ATOM	3670	CB	SER	B	109	-0.345	28.466	-14.642	1.00	17.76	
ATOM	3671	CG	SER	B	109	-0.427	27.508	-13.599	1.00	25.01	
ATOM	3672	C	SER	B	109	2.118	28.695	-14.290	1.00	15.55	
ATOM	3673	O	THR	B	110	2.547	27.799	-13.536	1.00	18.85	
ATOM	3674	N	THR	B	110	2.550	29.935	-14.259	1.00	13.95	
ATOM	3675	CA	THR	B	110	3.587	30.367	-13.332	1.00	14.07	
ATOM	3676	CB	THR	B	110	4.749	31.074	-14.088	1.00	15.61	
ATOM	3677	CG1	THR	B	110	4.262	32.260	-14.719	1.00	16.22	
ATOM	3678	CG2	THR	B	110	5.333	30.173	-15.168	1.00	13.87	
ATOM	3679	C	THR	B	110	3.081	31.376	-12.323	1.00	14.62	
ATOM	3680	O	LEU	B	111	2.028	32.023	-12.521	1.00	16.48	
ATOM	3681	N	LEU	B	111	3.835	31.498	-11.234	1.00	14.53	
ATOM	3682	CA	LEU	B	111	3.626	32.540	-10.236	1.00	14.82	
ATOM	3683	CB	LEU	B	111	3.048	31.999	-8.916	1.00	15.27	
ATOM	3684	CG	LEU	B	111	1.577	31.535	-8.991	1.00	16.13	
ATOM	3685	CD1	LEU	B	111	1.177	30.854	-7.706	1.00	15.76	
ATOM	3686	CD2	LEU	B	111	0.650	32.769	-9.243	1.00	15.24	
ATOM	3687	C	LEU	B	111	5.047	33.114	-10.070	1.00	16.26	
ATOM	3688	O	PRO	B	112	6.064	32.403	-10.174	1.00	16.00	
ATOM	3689	N	PRO	B	112	5.158	34.428	-9.873	1.00	15.54	
ATOM	3690	CA	PRO	B	112	4.031	35.374	-9.725	1.00	18.98	
ATOM	3691	CB	PRO	B	112	6.430	35.129	-9.711	1.00	16.92	
ATOM	3692	CG	PRO	B	112	5.984	36.546	-9.325	1.00	17.38	
ATOM	3693	C	PRO	B	112	4.697	36.676	-10.033	1.00	19.99	
ATOM	3694	O	PRO	B	112	7.388	34.571	-8.674	1.00	15.89	
ATOM	3695	N	ALA	B	113	6.978	34.259	-7.552	1.00	17.87	
ATOM	3696	CA	ALA	B	113	8.654	34.451	-9.066	1.00	17.65	
ATOM	3697	CB	ALA	B	113	9.702	33.993	-8.159	1.00	17.75	
ATOM	3698	CG	ALA	B	113	11.050	33.908	-8.901	1.00	18.59	
ATOM	3699	C	ALA	B	113	9.794	35.003	-6.997	1.00	19.95	
ATOM	3700	O	ALA	B	113	10.098	34.604	-5.873	1.00	18.56	
ATOM	3701	N	ALA	B	114	9.494	36.285	-7.254	1.00	19.88	
ATOM	3702	CA	ALA	B	114	9.546	37.297	-6.190	1.00	22.97	
ATOM	3703	CB	ALA	B	114	9.274	38.686	-6.762	1.00	24.68	
ATOM	3704	C	ALA	B	114	8.551	37.025	-5.073	1.00	24.13	
ATOM	3705	O	ASP	B	115	8.735	37.506	-3.948	1.00	25.27	
ATOM	3706	N	ASP	B	115	7.499	36.270	-5.374	1.00	22.97	
ATOM	3707	CA	ASP	B	115	6.458	35.936	-4.398	1.00	21.92	
ATOM	3708	CB	ASP	B	115	5.095	35.838	-5.085	1.00	25.25	
ATOM	3709	CG	ASP	B	115	4.653	37.144	-5.702	1.00	27.35	
ATOM	3710	OD1	ASP	B	115	5.197	38.200	-5.325	1.00	32.10	
ATOM	3711	OD2	ASP	B	115	3.756	37.115	-6.562	1.00	30.15	
ATOM	3712	C	ASP	B	115	6.686	34.620	-3.639	1.00	20.39	
ATOM	3713	O	PHE	B	116	5.892	34.256	-2.770	1.00	19.74	
ATOM	3714	N	PHE	B	116	7.743	33.883	-3.987	1.00	17.71	
ATOM	3715	CA	PHE	B	116	7.987	32.602	-3.323	1.00	18.38	
ATOM	3716	CB	PHE	B	116	9.004	31.796	-4.157	1.00	17.21	
ATOM	3717	CG	PHE	B	116	9.043	30.332	-3.810	1.00	18.03	
ATOM	3718	CD1	PHE	B	116	8.071	29.452	-4.300	1.00	16.40	
ATOM	3719	CD2	PHE	B	116	10.026	29.837	-2.955	1.00	17.20	
ATOM	3720	CE1	PHE	B	116	8.072	28.104	-3.949	1.00	18.94	
ATOM	3721	CE2	PHE	B	116	10.029	28.479	-2.596	1.00	15.80	
ATOM	3722	CZ	PHE	B	116	9.057	27.613	-3.091	1.00	18.24	
ATOM	3723	C	PHE	B	116	8.510	32.836	-1.896	1.00	18.89	
ATOM	3724	O	PRO	B	117	9.449	33.594	-1.716	1.00	19.05	
ATOM	3725	N	PRO	B	117	7.914	32.172	-0.888	1.00	20.37	
ATOM	3726	CA	PRO	B	117	6.913	31.117	-1.080	1.00	20.82	
ATOM	3727	CB	PRO	B	117	8.284	32.285	0.535	1.00	22.94	
ATOM	3728	CG	PRO	B	117	7.397	31.244	1.226	1.00	24.98	
ATOM	3729	C	PRO	B	117	6.285	30.991	0.290	1.00	22.83	
ATOM	3730	O	PRO	B	117	9.736	31.922	0.684	1.00	25.37	
ATOM	3731	N	ASN	B	118	10.204	31.012	0.018	1.00	26.02	
ATOM	3732	CA	ASN	B	118	10.441	32.630	1.556	1.00	27.41	
ATOM	3733	CB	ASN	B	118	11.857	32.398	1.767	1.00	30.63	
ATOM	3734	CG	ASN	B	118	12.638	33.537	1.081	1.00	34.20	
ATOM	3735	OD1	ASN	B	118	14.111	33.525	1.411	1.00	36.43	
ATOM	3736	OD2	ASN	B	118	14.518	33.929	2.500	1.00	39.71	
ATOM	3737	C	ASN	B	118	14.922	33.052	0.472	1.00	40.26	
ATOM	3738	O	ASN	B	118	12.103	32.399	3.275	1.00	31.98	
ATOM	3739	N	LEU	B	119	11.683	33.332	3.959	1.00	32.47	
ATOM	3740	CA	LEU	B	119	12.746	31.365	3.810	1.00	31.29	
ATOM	3741	CB	LEU	B	119	13.013	31.372	5.242	1.00	32.34	
ATOM	3742	CG	LEU	B	119	13.616	30.042	5.713	1.00	32.40	
ATOM	3743	CD1	LEU	B	119	12.712	28.820	5.889	1.00	34.29	
ATOM	3744	CD2	LEU	B	119	13.507	27.710	6.551	1.00	30.06	
ATOM	3745	C	LEU	B	119	11.516	29.170	6.758	1.00	32.87	
ATOM	3746	O	LEU	B	119	13.996	32.502	5.540	1.00	32.78	
ATOM	3747	N	ASP	B	120	14.922	32.751	4.767	1.00	33.27	
ATOM	3748	CA	ASP	B	120	13.785	33.170	6.668	1.00	35.53	
ATOM	3749	CB	ASP	B	120	14.634	34.264	7.106	1.00	38.51	
ATOM	3750	CG	ASP	B	120	14.100	34.820	8.442	1.00	41.15	
ATOM	3751	OD1	ASP	B	120	14.813	36.102	8.896	1.00	42.97	
ATOM	3752	OD2	ASP	B	120	15.288	36.880	8.032	1.00	41.78	
ATOM	3753	C	ASP	B	120	14.878	36.341	10.128	1.00	34.92	
ATOM	3754	O	ASP	B	120	16.076	33.793	7.240	1.00	33.81	
ATOM	3755	N	ASP	B	121	16.366	32.615	7.430	1.00	34.47	
ATOM	3756	CA	ASP	B	121	16.984	34.737	7.103	1.00	33.96	
ATOM	3757	CB	ASP	B	121	18.393	34.466	7.212	1.00	38.12	
ATOM	3758	CG	ASP	B	121	19.125	35.724	6.770	1.00	41.54	
ATOM	3759	OD1	ASP	B	121	18.471	36.339	5.540	1.00	42.91	
ATOM	3760	OD2	ASP	B	121	18.665	35.786	4.433	1.00	44.40	
ATOM	3761	C	ASP	B	121	17.730	37.344	5.687	1.00	31.06	
ATOM	3762	O	ASP	B	121	18.648	34.144	8.672	1.00	30.33	
ATOM	3763	N	TRP	B	122	17.935	34.611	9.549	1.00	29.45	
ATOM	3764	CA	TRP	B	122	19.642	33.314	8.927	1.00	26.54	
ATOM	3765	CB	TRP	B	122	19.953	32.969	10.301	1.00		

Figure 1 (continued 38)

ATOM	3766	CB	TRP	B	122	19.021	31.833	10.766	1.00	24.27	B
ATOM	3767	CG	TRP	B	122	19.072	30.629	9.899	1.00	23.67	B
ATOM	3768	CD2	TRP	B	122	19.832	29.445	10.127	1.00	23.03	B
ATOM	3769	CE2	TRP	B	122	19.617	28.587	9.027	1.00	24.46	B
ATOM	3770	CE3	TRP	B	122	20.680	29.020	11.157	1.00	21.61	B
ATOM	3771	CD1	TRP	B	122	18.435	30.451	8.697	1.00	25.67	B
ATOM	3772	NE1	TRP	B	122	18.760	29.225	8.167	1.00	25.03	B
ATOM	3773	CZ2	TRP	B	122	20.224	27.327	8.929	1.00	24.86	B
ATOM	3774	CZ3	TRP	B	122	21.276	27.769	11.061	1.00	21.60	B
ATOM	3775	CH2	TRP	B	122	21.047	26.940	9.956	1.00	25.02	B
ATOM	3776	C	TRP	B	122	21.416	32.581	10.381	1.00	25.76	B
ATOM	3777	O	TRP	B	122	22.081	32.419	9.354	1.00	25.40	B
ATOM	3778	N	GLN	B	123	21.932	32.437	11.600	1.00	22.86	B
ATOM	3779	CA	GLN	B	123	23.330	32.106	11.786	1.00	25.29	B
ATOM	3780	CB	GLN	B	123	23.960	33.225	12.614	1.00	23.33	B
ATOM	3781	CG	GLN	B	123	23.736	34.611	12.017	1.00	28.45	B
ATOM	3782	CD	GLN	B	123	24.576	34.837	10.772	1.00	28.70	B
ATOM	3783	OE1	GLN	B	123	24.445	35.856	10.099	1.00	32.60	B
ATOM	3784	NE2	GLN	B	123	25.447	33.889	10.469	1.00	32.57	B
ATOM	3785	C	GLN	B	123	23.537	30.762	12.492	1.00	24.00	B
ATOM	3786	O	GLN	B	123	22.879	30.502	13.494	1.00	25.77	B
ATOM	3787	N	SER	B	124	24.440	29.917	11.994	1.00	23.58	B
ATOM	3788	CA	SER	B	124	24.680	28.643	12.680	1.00	24.40	B
ATOM	3789	CB	SER	B	124	25.295	27.574	11.778	1.00	26.13	B
ATOM	3790	OG	SER	B	124	26.636	27.883	11.441	1.00	32.13	B
ATOM	3791	C	SER	B	124	25.600	28.849	13.870	1.00	24.43	B
ATOM	3792	O	SER	B	124	26.566	29.622	13.803	1.00	24.71	B
ATOM	3793	N	GLU	B	125	25.274	28.155	14.952	1.00	23.06	B
ATOM	3794	CA	GLU	B	125	26.035	28.205	16.203	1.00	24.57	B
ATOM	3795	CB	GLU	B	125	25.093	28.516	17.360	1.00	25.73	B
ATOM	3796	CG	GLU	B	125	24.399	29.857	17.254	1.00	32.47	B
ATOM	3797	CD	GLU	B	125	23.353	30.051	18.344	1.00	35.90	B
ATOM	3798	OE1	GLU	B	125	23.423	29.345	19.381	1.00	39.08	B
ATOM	3799	OE2	GLU	B	125	22.464	30.912	18.168	1.00	39.18	B
ATOM	3800	C	GLU	B	125	26.786	26.907	16.508	1.00	24.50	B
ATOM	3801	O	GLU	B	125	27.665	26.879	17.382	1.00	24.43	B
ATOM	3802	N	VAL	B	126	26.419	25.815	15.844	1.00	22.81	B
ATOM	3803	CA	VAL	B	126	27.106	24.539	16.031	1.00	24.05	B
ATOM	3804	CB	VAL	B	126	26.434	23.637	17.119	1.00	24.27	B
ATOM	3805	CG1	VAL	B	126	25.027	23.339	16.751	1.00	25.14	B
ATOM	3806	CG2	VAL	B	126	27.216	22.320	17.271	1.00	27.01	B
ATOM	3807	C	VAL	B	126	27.078	23.835	14.690	1.00	23.78	B
ATOM	3808	O	VAL	B	126	26.073	23.885	13.967	1.00	24.92	B
ATOM	3809	N	GLU	B	127	28.182	23.193	14.344	1.00	22.15	B
ATOM	3810	CA	GLU	B	127	28.281	22.509	13.081	1.00	21.91	B
ATOM	3811	CB	GLU	B	127	29.002	23.394	12.051	1.00	23.10	B
ATOM	3812	CG	GLU	B	127	28.426	24.768	11.966	1.00	26.12	B
ATOM	3813	CD	GLU	B	127	29.056	25.636	10.884	1.00	27.63	B
ATOM	3814	OE1	GLU	B	127	28.434	26.672	10.546	1.00	27.53	B
ATOM	3815	OE2	GLU	B	127	30.157	25.298	10.403	1.00	28.31	B
ATOM	3816	C	GLU	B	127	29.069	21.240	13.254	1.00	21.48	B
ATOM	3817	O	GLU	B	127	30.034	21.189	14.027	1.00	22.56	B
ATOM	3818	N	PHE	B	128	28.665	20.215	12.536	1.00	20.20	B
ATOM	3819	CA	PHE	B	128	29.377	18.956	12.576	1.00	19.84	B
ATOM	3820	CB	PHE	B	128	29.096	18.211	13.895	1.00	21.34	B
ATOM	3821	CG	PHE	B	128	27.632	18.001	14.172	1.00	19.59	B
ATOM	3822	CD1	PHE	B	128	26.892	18.969	14.829	1.00	20.54	B
ATOM	3823	CD2	PHE	B	128	26.993	16.851	13.729	1.00	19.54	B
ATOM	3824	CE1	PHE	B	128	25.516	18.802	15.043	1.00	18.79	B
ATOM	3825	CE2	PHE	B	128	25.616	16.672	13.938	1.00	20.56	B
ATOM	3826	CZ	PHE	B	128	24.886	17.646	14.591	1.00	20.20	B
ATOM	3827	C	PHE	B	128	28.997	18.096	11.392	1.00	21.44	B
ATOM	3828	O	PHE	B	128	27.986	18.338	10.707	1.00	19.41	B
ATOM	3829	N	THR	B	129	29.836	17.110	11.111	1.00	19.99	B
ATOM	3830	CA	THR	B	129	29.562	16.198	10.029	1.00	22.84	B
ATOM	3831	CB	THR	B	129	30.712	16.238	8.982	1.00	25.69	B
ATOM	3832	OG1	THR	B	129	31.949	15.897	9.626	1.00	32.56	B
ATOM	3833	CG2	THR	B	129	30.846	17.633	8.404	1.00	25.73	B
ATOM	3834	C	THR	B	129	29.415	14.792	10.608	1.00	24.49	B
ATOM	3835	O	THR	B	129	30.021	14.476	11.630	1.00	26.37	B
ATOM	3836	N	LEU	B	130	28.577	13.964	10.000	1.00	24.49	B
ATOM	3837	CA	LEU	B	130	28.423	12.589	10.477	1.00	24.08	B
ATOM	3838	CB	LEU	B	130	27.407	12.505	11.633	1.00	25.54	B
ATOM	3839	CG	LEU	B	130	25.900	12.579	11.337	1.00	25.32	B
ATOM	3840	CD1	LEU	B	130	25.149	12.111	12.598	1.00	24.84	B
ATOM	3841	CD2	LEU	B	130	25.477	13.989	10.960	1.00	23.86	B
ATOM	3842	C	LEU	B	130	27.965	11.707	9.327	1.00	23.70	B
ATOM	3843	O	LEU	B	130	27.413	12.191	8.343	1.00	23.84	B
ATOM	3844	N	PRO	B	131	28.197	10.389	9.425	1.00	23.64	B
ATOM	3845	CD	PRO	B	131	28.932	9.700	10.501	1.00	22.59	B
ATOM	3846	CA	PRO	B	131	27.790	9.465	8.371	1.00	22.27	B
ATOM	3847	CB	PRO	B	131	28.311	8.105	8.871	1.00	23.69	B
ATOM	3848	CG	PRO	B	131	29.456	8.479	9.793	1.00	23.88	B
ATOM	3849	C	PRO	B	131	26.273	9.459	8.237	1.00	23.45	B
ATOM	3850	O	PRO	B	131	25.555	9.578	9.239	1.00	21.35	B
ATOM	3851	N	GLN	B	132	25.778	9.341	7.013	1.00	22.22	B
ATOM	3852	CA	GLN	B	132	24.337	9.290	6.833	1.00	24.38	B
ATOM	3853	CB	GLN	B	132	23.975	9.060	5.383	1.00	27.52	B
ATOM	3854	CG	GLN	B	132	24.306	10.174	4.466	1.00	30.36	B
ATOM	3855	CD	GLN	B	132	23.834	9.867	3.061	1.00	32.41	B
ATOM	3856	OE1	GLN	B	132	22.667	9.539	2.845	1.00	34.45	B
ATOM	3857	NE2	GLN	B	132	24.736	9.964	2.100	1.00	33.22	B
ATOM	3858	C	GLN	B	132	23.737	8.134	7.642	1.00	24.58	B
ATOM	3859	O	GLN	B	132	22.646	8.253	8.187	1.00	23.73	B
ATOM	3860	N	ALA	B	133	24.446	7.005	7.692	1.00	24.46	B
ATOM	3861	CA	ALA	B	133	23.940	5.844	8.416	1.00	23.74	B
ATOM	3862	CB	ALA	B	133	24.911	4.650	8.241	1.00	25.48	B
ATOM	3863	C	ALA	B	133	23.677	6.103	9.896	1.00	22.24	B
ATOM	3864	O	ALA	B	133	22.768	5.493	10.482	1.00	23.23	B
ATOM	3865	N	THR	B	134	24.470	6.976	10.498	1.00	21.71	B

Figure 1 (continued 39)

ATOM	3866	CA	THR	B	134	24.329	7.337	11.906	1.00	21.35
ATOM	3867	CB	THR	B	134	25.520	8.155	12.368	1.00	23.54
ATOM	3868	OG1	THR	B	134	26.705	7.376	12.169	1.00	25.66
ATOM	3869	CG2	THR	B	134	25.375	8.570	13.822	1.00	22.93
ATOM	3870	C	THR	B	134	23.077	8.161	12.089	1.00	20.95
ATOM	3871	O	THR	B	134	22.329	7.988	13.053	1.00	20.93
ATOM	3872	N	MET	B	135	22.855	9.097	11.172	1.00	19.95
ATOM	3873	CA	MET	B	135	21.654	9.897	11.284	1.00	20.19
ATOM	3874	CB	MET	B	135	21.626	10.994	10.222	1.00	20.76
ATOM	3875	CG	MET	B	135	20.385	11.886	10.326	1.00	22.47
ATOM	3876	SD	MET	B	135	20.158	12.699	11.928	1.00	25.83
ATOM	3877	CE	MET	B	135	21.360	14.018	11.870	1.00	26.97
ATOM	3878	C	MET	B	135	20.442	8.986	11.114	1.00	18.60
ATOM	3879	O	MET	B	135	19.453	9.134	11.831	1.00	18.63
ATOM	3880	N	LYS	B	136	20.487	8.053	10.169	1.00	19.85
ATOM	3881	CA	LYS	B	136	19.356	7.155	9.976	1.00	21.55
ATOM	3882	CB	LYS	B	136	19.595	6.173	8.831	1.00	24.24
ATOM	3883	CG	LYS	B	136	18.382	5.263	8.598	1.00	25.85
ATOM	3884	CD	LYS	B	136	18.333	4.703	7.182	1.00	32.16
ATOM	3885	CE	LYS	B	136	19.291	3.541	7.025	1.00	33.18
ATOM	3886	NZ	LYS	B	136	18.863	2.381	7.861	1.00	36.66
ATOM	3887	C	LYS	B	136	19.092	6.348	11.249	1.00	22.36
ATOM	3888	O	LYS	B	136	17.957	6.211	11.685	1.00	21.54
ATOM	3889	N	ARG	B	137	20.154	5.791	11.819	1.00	21.72
ATOM	3890	CA	ARG	B	137	20.004	4.998	13.037	1.00	21.93
ATOM	3891	CB	ARG	B	137	21.368	4.481	13.501	1.00	24.73
ATOM	3892	CG	ARG	B	137	21.339	3.432	14.643	1.00	28.08
ATOM	3893	CD	ARG	B	137	21.297	4.069	16.012	1.00	30.79
ATOM	3894	NE	ARG	B	137	21.609	3.129	17.104	1.00	31.38
ATOM	3895	CZ	ARG	B	137	20.802	2.161	17.547	1.00	31.74
ATOM	3896	NH1	ARG	B	137	19.604	1.962	17.003	1.00	31.80
ATOM	3897	NH2	ARG	B	137	21.184	1.411	18.578	1.00	29.88
ATOM	3898	C	ARG	B	137	19.360	5.820	14.141	1.00	20.76
ATOM	3899	O	ARG	B	137	18.389	5.386	14.770	1.00	21.28
ATOM	3900	N	LEU	B	138	19.880	7.021	14.364	1.00	19.03
ATOM	3901	CA	LEU	B	138	19.355	7.902	15.415	1.00	17.43
ATOM	3902	CB	LEU	B	138	20.123	9.223	15.421	1.00	17.77
ATOM	3903	CG	LEU	B	138	21.500	9.129	16.066	1.00	18.25
ATOM	3904	CD1	LEU	B	138	22.325	10.379	15.773	1.00	18.28
ATOM	3905	CD2	LEU	B	138	21.330	8.948	17.581	1.00	18.59
ATOM	3906	C	LEU	B	138	17.875	8.209	15.283	1.00	19.04
ATOM	3907	O	LEU	B	138	17.130	8.236	16.291	1.00	17.18
ATOM	3908	N	ILE	B	139	17.436	8.467	14.055	1.00	16.38
ATOM	3909	CA	ILE	B	139	16.027	8.783	13.843	1.00	16.79
ATOM	3910	CB	ILE	B	139	15.811	9.516	12.479	1.00	16.68
ATOM	3911	CG2	ILE	B	139	14.322	9.634	12.168	1.00	20.18
ATOM	3912	CG1	ILE	B	139	16.478	10.883	12.561	1.00	18.34
ATOM	3913	CD1	ILE	B	139	16.478	11.689	11.221	1.00	19.90
ATOM	3914	C	ILE	B	139	15.143	7.553	13.916	1.00	16.56
ATOM	3915	O	ILE	B	139	14.128	7.563	14.590	1.00	16.80
ATOM	3916	N	GLU	B	140	15.526	6.482	13.238	1.00	15.42
ATOM	3917	CA	GLU	B	140	14.720	5.276	13.263	1.00	16.12
ATOM	3918	CB	GLU	B	140	15.316	4.232	12.322	1.00	17.99
ATOM	3919	CG	GLU	B	140	15.176	4.640	10.858	1.00	22.86
ATOM	3920	CD	GLU	B	140	15.372	3.489	9.890	1.00	27.30
ATOM	3921	OE1	GLU	B	140	16.289	2.678	10.103	1.00	28.72
ATOM	3922	OE2	GLU	B	140	14.609	3.402	8.905	1.00	31.19
ATOM	3923	C	GLU	B	140	14.595	4.687	14.676	1.00	15.11
ATOM	3924	O	GLU	B	140	13.591	4.042	15.003	1.00	17.70
ATOM	3925	N	ALA	B	141	15.609	4.903	15.503	1.00	15.65
ATOM	3926	CA	ALA	B	141	15.577	4.336	16.849	1.00	15.07
ATOM	3927	CB	ALA	B	141	16.963	4.469	17.487	1.00	18.37
ATOM	3928	C	ALA	B	141	14.530	5.000	17.751	1.00	14.92
ATOM	3929	O	ALA	B	141	14.080	4.409	18.734	1.00	14.51
ATOM	3930	N	THR	B	142	14.097	6.209	17.401	1.00	13.57
ATOM	3931	CA	THR	B	142	13.205	6.922	18.309	1.00	13.58
ATOM	3932	CB	THR	B	142	13.994	8.081	18.978	1.00	17.09
ATOM	3933	OG1	THR	B	142	14.329	9.057	17.962	1.00	17.94
ATOM	3934	CG2	THR	B	142	15.336	7.553	15.627	1.00	15.55
ATOM	3935	C	THR	B	142	11.943	7.507	17.706	1.00	14.63
ATOM	3936	O	THR	B	142	11.004	7.820	18.438	1.00	13.14
ATOM	3937	N	GLN	B	143	11.899	7.640	16.381	1.00	13.61
ATOM	3938	CA	GLN	B	143	10.752	8.313	15.743	1.00	15.74
ATOM	3939	CB	GLN	B	143	10.937	8.285	14.215	1.00	17.04
ATOM	3940	CG	GLN	B	143	9.799	8.931	13.418	1.00	18.95
ATOM	3941	CD	GLN	B	143	10.073	8.886	11.922	1.00	22.30
ATOM	3942	OE1	GLN	B	143	10.552	7.873	11.411	1.00	23.43
ATOM	3943	NE2	GLN	B	143	9.769	9.989	11.211	1.00	23.11
ATOM	3944	C	GLN	B	143	9.380	7.797	16.137	1.00	15.74
ATOM	3945	O	GLN	B	143	8.438	8.577	16.322	1.00	17.49
ATOM	3946	N	PHE	B	144	9.254	6.489	16.319	1.00	15.47
ATOM	3947	CA	PHE	B	144	7.951	5.942	16.640	1.00	15.79
ATOM	3948	CB	PHE	B	144	8.009	4.408	16.623	1.00	16.45
ATOM	3949	CG	PHE	B	144	8.745	3.818	17.785	1.00	15.61
ATOM	3950	CD1	PHE	B	144	10.129	3.644	17.740	1.00	14.87
ATOM	3951	CD2	PHE	B	144	8.052	3.490	18.952	1.00	15.49
ATOM	3952	CE1	PHE	B	144	10.825	3.158	18.849	1.00	14.78
ATOM	3953	CE2	PHE	B	144	8.730	3.002	20.072	1.00	14.34
ATOM	3954	CZ	PHE	B	144	10.108	2.836	20.033	1.00	15.36
ATOM	3955	C	PHE	B	144	7.390	6.402	17.979	1.00	16.39
ATOM	3956	O	PHE	B	144	6.196	6.252	18.206	1.00	16.31
ATOM	3957	N	SER	B	145	8.233	6.932	18.857	1.00	15.52
ATOM	3958	CA	SER	B	145	7.765	7.357	20.178	1.00	15.49
ATOM	3959	CB	SER	B	145	8.842	7.137	21.236	1.00	19.43
ATOM	3960	OG	SER	B	145	9.051	5.743	21.459	1.00	19.03
ATOM	3961	C	SER	B	145	7.321	8.812	20.231	1.00	17.97
ATOM	3962	O	SER	B	145	6.983	9.307	21.325	1.00	17.36
ATOM	3963	N	MET	B	146	7.362	9.507	19.093	1.00	17.94
ATOM	3964	CA	MET	B	146	6.910	10.907	19.066	1.00	19.19
ATOM	3965	CB	MET	B	146	7.260	11.560	17.711	1.00	21.36

Figure 1 (continued 40)

ATOM	3966	CG	MET	B	146	8.716	11.608	17.434	1.00	19.66	B
ATOM	3967	SD	MET	B	146	8.961	11.941	15.674	1.00	23.93	B
ATOM	3968	CE	MET	B	146	8.838	13.621	15.659	1.00	23.07	B
ATOM	3969	C	MET	B	146	5.393	10.948	19.237	1.00	19.89	B
ATOM	3970	O	MET	B	146	4.683	10.038	18.798	1.00	21.24	B
ATOM	3971	N	ALA	B	147	4.879	12.014	19.853	1.00	21.60	B
ATOM	3972	CA	ALA	B	147	3.438	12.137	20.009	1.00	24.00	B
ATOM	3973	CB	ALA	B	147	3.112	13.270	21.028	1.00	23.97	B
ATOM	3974	C	ALA	B	147	2.775	12.439	18.661	1.00	25.73	B
ATOM	3975	O	ALA	B	147	3.433	12.878	17.714	1.00	23.85	B
ATOM	3976	N	HIS	B	148	1.473	12.184	18.568	1.00	30.66	B
ATOM	3977	CA	HIS	B	148	0.719	12.469	17.348	1.00	34.48	B
ATOM	3978	CB	HIS	B	148	0.020	11.211	16.829	1.00	37.35	B
ATOM	3979	CG	HIS	B	148	0.944	10.060	16.595	1.00	40.57	B
ATOM	3980	CD2	HIS	B	148	0.913	8.786	17.053	1.00	41.90	B
ATOM	3981	ND1	HIS	B	148	2.056	10.150	15.783	1.00	42.40	B
ATOM	3982	CE1	HIS	B	148	2.672	8.981	15.754	1.00	42.24	B
ATOM	3983	NE2	HIS	B	148	1.998	8.136	16.515	1.00	43.11	B
ATOM	3984	C	HIS	B	148	-0.344	13.519	17.668	1.00	36.54	B
ATOM	3985	O	HIS	B	148	-1.386	13.201	18.262	1.00	36.38	B
ATOM	3986	N	GLN	B	149	-0.078	14.761	17.281	1.00	37.77	B
ATOM	3987	CA	GLN	B	149	-1.019	15.853	17.523	1.00	39.65	B
ATOM	3988	CB	GLN	B	149	-2.290	15.638	16.680	1.00	41.57	B
ATOM	3989	CG	GLN	B	149	-2.022	15.462	15.185	1.00	44.91	B
ATOM	3990	CD	GLN	B	149	-3.278	15.215	14.355	1.00	46.65	B
ATOM	3991	OE1	GLN	B	149	-4.068	14.320	14.648	1.00	48.28	B
ATOM	3992	NE2	GLN	B	149	-3.453	16.003	13.300	1.00	48.05	B
ATOM	3993	C	GLN	B	149	-1.376	15.995	19.005	1.00	39.02	B
ATOM	3994	O	GLN	B	149	-2.558	16.067	19.370	1.00	40.48	B
ATOM	3995	N	ASP	B	150	-0.354	16.029	19.857	1.00	38.46	B
ATOM	3996	CA	ASP	B	150	0.679	16.192	21.299	1.00	37.30	B
ATOM	3997	CB	ASP	B	150	0.445	15.640	22.059	1.00	37.60	B
ATOM	3998	CG	ASP	B	150	0.093	15.547	23.561	1.00	38.25	B
ATOM	3999	OD1	ASP	B	150	0.621	16.575	24.172	1.00	37.98	B
ATOM	4000	OD2	ASP	B	150	-0.673	14.450	24.149	1.00	38.03	B
ATOM	4001	C	ASP	B	150	-0.191	17.695	21.578	1.00	35.91	B
ATOM	4002	O	ASP	B	150	-1.325	18.526	20.803	1.00	38.58	B
ATOM	4003	N	VAL	B	151	-1.527	18.036	22.687	1.00	38.83	B
ATOM	4004	CA	VAL	B	151	-2.403	19.432	23.055	1.00	39.52	B
ATOM	4005	CB	VAL	B	151	-2.705	19.567	24.316	1.00	39.97	B
ATOM	4006	CG1	VAL	B	151	-3.678	21.028	24.579	1.00	40.52	B
ATOM	4007	CG2	VAL	B	151	-0.185	18.778	24.142	1.00	38.33	B
ATOM	4008	C	VAL	B	151	0.047	20.057	23.331	1.00	38.42	B
ATOM	4009	O	VAL	B	151	0.676	19.302	24.012	1.00	37.29	B
ATOM	4010	N	ARG	B	152	2.022	19.761	24.291	1.00	36.95	B
ATOM	4011	CA	ARG	B	152	2.718	18.842	25.304	1.00	38.55	B
ATOM	4012	CB	ARG	B	152	2.144	18.896	26.717	1.00	40.64	B
ATOM	4013	CG	ARG	B	152	0.984	17.935	26.875	1.00	41.39	B
ATOM	4014	CD	ARG	B	152	1.454	16.561	27.041	1.00	43.21	B
ATOM	4015	NE	ARG	B	152	0.674	15.492	26.935	1.00	44.44	B
ATOM	4016	CZ	ARG	B	152	-0.619	15.645	26.656	1.00	46.42	B
ATOM	4017	NH1	ARG	B	152	1.176	14.274	27.116	1.00	43.86	B
ATOM	4018	NH2	ARG	B	152	2.683	19.626	22.921	1.00	36.41	B
ATOM	4019	C	ARG	B	152	3.410	18.659	22.678	1.00	34.83	B
ATOM	4020	O	ARG	B	152	2.403	20.580	22.031	1.00	34.80	B
ATOM	4021	N	TYR	B	153	2.927	20.555	20.665	1.00	33.74	B
ATOM	4022	CA	TYR	B	153	2.686	21.906	19.963	1.00	35.98	B
ATOM	4023	CB	TYR	B	153	3.406	23.061	20.611	1.00	38.54	B
ATOM	4024	CG	TYR	B	153	2.975	23.581	21.835	1.00	39.34	B
ATOM	4025	CD1	TYR	B	153	3.698	24.581	22.487	1.00	39.67	B
ATOM	4026	CE1	TYR	B	153	4.574	23.582	20.049	1.00	39.01	B
ATOM	4027	CD2	TYR	B	153	5.310	24.586	20.696	1.00	39.82	B
ATOM	4028	CE2	TYR	B	153	4.866	25.075	21.915	1.00	40.12	B
ATOM	4029	CZ	TYR	B	153	5.607	26.030	22.574	1.00	39.51	B
ATOM	4030	OH	TYR	B	153	4.403	20.171	20.568	1.00	32.24	B
ATOM	4031	C	TYR	B	153	4.833	19.616	19.554	1.00	30.69	B
ATOM	4032	O	TYR	B	153	5.175	20.445	21.612	1.00	30.25	B
ATOM	4033	N	TYR	B	154	6.585	20.103	21.597	1.00	30.50	B
ATOM	4034	CA	TYR	B	154	7.324	20.751	22.779	1.00	32.66	B
ATOM	4035	CB	TYR	B	154	6.785	20.471	24.172	1.00	35.85	B
ATOM	4036	CG	TYR	B	154	7.325	19.450	24.953	1.00	36.54	B
ATOM	4037	CD1	TYR	B	154	6.888	19.225	26.267	1.00	37.57	B
ATOM	4038	CE1	TYR	B	154	5.779	21.270	24.734	1.00	37.28	B
ATOM	4039	CD2	TYR	B	154	5.334	21.053	26.047	1.00	37.15	B
ATOM	4040	CE2	TYR	B	154	5.895	20.030	26.805	1.00	38.13	B
ATOM	4041	CZ	TYR	B	154	5.477	19.804	28.098	1.00	38.78	B
ATOM	4042	OH	TYR	B	154	6.813	18.585	21.571	1.00	29.59	B
ATOM	4043	C	TYR	B	154	7.817	18.113	21.040	1.00	28.98	B
ATOM	4044	O	TYR	B	154	5.874	17.816	22.109	1.00	27.11	B
ATOM	4045	N	LEU	B	155	6.029	16.359	22.087	1.00	26.11	B
ATOM	4046	CA	LEU	B	155	5.055	15.686	23.064	1.00	25.90	B
ATOM	4047	CB	LEU	B	155	5.260	16.046	24.536	1.00	27.10	B
ATOM	4048	CG	LEU	B	155	4.256	15.237	25.360	1.00	29.20	B
ATOM	4049	CD1	LEU	B	155	6.686	15.757	24.980	1.00	28.73	B
ATOM	4050	CD2	LEU	B	155	5.808	15.776	20.682	1.00	25.64	B
ATOM	4051	C	LEU	B	155	6.177	14.613	20.431	1.00	25.89	B
ATOM	4052	O	LEU	B	155	5.210	16.560	19.781	1.00	23.01	B
ATOM	4053	N	ASN	B	156	4.962	16.121	18.405	1.00	23.44	B
ATOM	4054	CA	ASN	B	156	3.911	16.986	17.737	1.00	25.76	B
ATOM	4055	CB	ASN	B	156	2.570	16.900	18.436	1.00	29.20	B
ATOM	4056	CG	ASN	B	156	1.720	17.790	18.296	1.00	30.71	B
ATOM	4057	OD1	ASN	B	156	2.373	15.830	19.194	1.00	24.28	B
ATOM	4058	ND2	ASN	B	156	6.235	16.141	17.547	1.00	23.66	B
ATOM	4059	C	ASN	B	156	6.203	15.696	16.400	1.00	23.58	B
ATOM	4060	O	ASN	B	156	7.332	16.630	18.122	1.00	22.86	B
ATOM	4061	N	GLY	B	157	8.596	16.686	17.399	1.00	22.29	B
ATOM	4062	CA	GLY	B	157	9.630	15.756	18.000	1.00	22.40	B
ATOM	4063	C	GLY	B	157	9.307	14.894	18.819	1.00	21.77	B
ATOM	4064	O	GLY	B	157	10.890	15.911	17.604	1.00	19.12	B
ATOM	4065	N	MET	B	158						B

Figure 1 (continued 41)

[illegible]

Figure 1 (continued 42)

ATOM	4166	CA	VAL	B	170	14.796	11.705	22.176	1.00	18.28	B
ATOM	4167	CB	VAL	B	170	15.031	12.497	23.489	1.00	17.76	B
ATOM	4168	CG1	VAL	B	170	14.085	11.948	24.589	1.00	18.88	B
ATOM	4169	CG2	VAL	B	170	16.520	12.397	23.913	1.00	18.42	B
ATOM	4170	C	VAL	B	170	13.368	11.981	21.674	1.00	18.46	B
ATOM	4171	O	VAL	B	170	13.087	13.010	21.060	1.00	18.89	B
ATOM	4172	N	ALA	B	171	12.455	11.031	21.908	1.00	15.83	B
ATOM	4173	CA	ALA	B	171	11.069	11.206	21.518	1.00	16.19	B
ATOM	4174	CB	ALA	B	171	10.771	10.503	20.212	1.00	16.47	B
ATOM	4175	C	ALA	B	171	10.234	10.606	22.617	1.00	17.41	B
ATOM	4176	O	ALA	B	171	10.642	9.616	23.213	1.00	18.10	B
ATOM	4177	N	THR	B	172	9.112	11.246	22.902	1.00	16.52	B
ATOM	4178	CA	THR	B	172	8.212	10.730	23.917	1.00	17.52	B
ATOM	4179	CB	THR	B	172	8.776	11.014	25.344	1.00	18.95	B
ATOM	4180	CG1	THR	B	172	7.931	10.400	26.328	1.00	19.33	B
ATOM	4181	CG2	THR	B	172	8.870	12.532	25.619	1.00	18.29	B
ATOM	4182	C	THR	B	172	6.805	11.269	23.709	1.00	18.84	B
ATOM	4183	O	THR	B	172	6.588	12.352	23.145	1.00	20.21	B
ATOM	4184	N	ASP	B	173	5.820	10.481	24.134	1.00	18.12	B
ATOM	4185	CA	ASP	B	173	4.447	10.902	23.972	1.00	19.17	B
ATOM	4186	CB	ASP	B	173	3.709	9.980	22.996	1.00	19.41	B
ATOM	4187	CG	ASP	B	173	3.663	8.531	23.461	1.00	19.37	B
ATOM	4188	OD1	ASP	B	173	4.197	8.212	24.540	1.00	20.26	B
ATOM	4189	OD2	ASP	B	173	3.087	7.712	22.710	1.00	18.53	B
ATOM	4190	C	ASP	B	173	3.766	10.895	25.336	1.00	19.52	B
ATOM	4191	O	ASP	B	173	2.546	11.011	25.408	1.00	22.02	B
ATOM	4192	N	GLY	B	174	4.562	10.770	26.397	1.00	20.37	B
ATOM	4193	CA	GLY	B	174	3.992	10.745	27.737	1.00	22.96	B
ATOM	4194	C	GLY	B	174	3.762	9.337	28.266	1.00	24.51	B
ATOM	4195	O	GLY	B	174	3.667	9.141	29.489	1.00	26.84	B
ATOM	4196	N	HIS	B	175	3.650	8.349	27.375	1.00	23.92	B
ATOM	4197	CA	HIS	B	175	3.440	6.953	27.796	1.00	22.95	B
ATOM	4198	CB	HIS	B	175	2.313	6.309	26.977	1.00	25.89	B
ATOM	4199	CG	HIS	B	175	0.992	6.997	27.119	1.00	28.87	B
ATOM	4200	CD2	HIS	B	175	0.106	7.435	26.193	1.00	30.90	B
ATOM	4201	ND1	HIS	B	175	0.420	7.255	28.345	1.00	30.54	B
ATOM	4202	CE1	HIS	B	175	-0.763	7.817	28.170	1.00	28.94	B
ATOM	4203	NE2	HIS	B	175	-0.977	7.938	26.875	1.00	31.49	B
ATOM	4204	C	HIS	B	175	4.706	6.135	27.641	1.00	23.03	B
ATOM	4205	O	HIS	B	175	4.990	5.212	28.403	1.00	22.08	B
ATOM	4206	N	ARG	B	176	5.461	6.461	26.617	1.00	18.76	B
ATOM	4207	CA	ARG	B	176	6.711	5.768	26.422	1.00	18.30	B
ATOM	4208	CB	ARG	B	176	6.575	4.633	25.398	1.00	19.53	B
ATOM	4209	CG	ARG	B	176	6.329	5.094	23.954	1.00	22.88	B
ATOM	4210	CD	ARG	B	176	4.876	4.888	23.657	1.00	22.11	B
ATOM	4211	NE	ARG	B	176	4.435	5.312	22.314	1.00	22.09	B
ATOM	4212	CZ	ARG	B	176	4.555	4.591	21.202	1.00	20.17	B
ATOM	4213	NH1	ARG	B	176	5.159	3.403	21.213	1.00	17.04	B
ATOM	4214	NH2	ARG	B	176	3.914	4.977	20.120	1.00	20.02	B
ATOM	4215	C	ARG	B	176	7.684	6.807	25.902	1.00	17.30	B
ATOM	4216	O	ARG	B	176	7.255	7.860	25.374	1.00	18.10	B
ATOM	4217	N	LEU	B	177	8.957	6.504	26.080	1.00	17.97	B
ATOM	4218	CA	LEU	B	177	10.049	7.360	25.633	1.00	17.85	B
ATOM	4219	CB	LEU	B	177	10.664	8.095	26.827	1.00	18.29	B
ATOM	4220	CG	LEU	B	177	11.921	8.955	26.611	1.00	16.28	B
ATOM	4221	CD1	LEU	B	177	11.819	10.163	27.559	1.00	19.52	B
ATOM	4222	CD2	LEU	B	177	13.191	8.172	26.839	1.00	19.12	B
ATOM	4223	C	LEU	B	177	11.110	6.517	24.964	1.00	18.45	B
ATOM	4224	O	LEU	B	177	11.291	5.329	25.281	1.00	18.33	B
ATOM	4225	N	ALA	B	178	11.801	7.131	24.006	1.00	15.84	B
ATOM	4226	CA	ALA	B	178	12.899	6.489	23.308	1.00	15.12	B
ATOM	4227	CB	ALA	B	178	12.495	6.133	21.883	1.00	13.82	B
ATOM	4228	C	ALA	B	178	14.041	7.488	23.279	1.00	15.48	B
ATOM	4229	O	ALA	B	178	13.797	8.670	23.063	1.00	17.09	B
ATOM	4230	N	VAL	B	179	15.258	7.014	23.546	1.00	17.40	B
ATOM	4231	CA	VAL	B	179	16.470	7.851	23.508	1.00	18.38	B
ATOM	4232	CB	VAL	B	179	16.881	8.318	24.937	1.00	18.67	B
ATOM	4233	CG1	VAL	B	179	17.294	7.120	25.770	1.00	19.18	B
ATOM	4234	CG2	VAL	B	179	18.060	9.286	24.864	1.00	20.37	B
ATOM	4235	C	VAL	B	179	17.590	7.037	22.849	1.00	19.44	B
ATOM	4236	O	VAL	B	179	17.737	5.829	23.092	1.00	19.37	B
ATOM	4237	N	CYS	B	180	18.370	7.676	21.968	1.00	17.08	B
ATOM	4238	CA	CYS	B	180	19.434	6.979	21.293	1.00	18.58	B
ATOM	4239	CB	CYS	B	180	18.961	6.489	19.918	1.00	17.06	B
ATOM	4240	SG	CYS	B	180	20.198	5.643	18.973	1.00	22.31	B
ATOM	4241	C	CYS	B	180	20.602	7.948	21.135	1.00	19.35	B
ATOM	4242	O	CYS	B	180	20.405	9.093	20.736	1.00	19.68	B
ATOM	4243	N	SER	B	181	21.798	7.464	21.442	1.00	21.74	B
ATOM	4244	CA	SER	B	181	23.015	8.277	21.359	1.00	25.46	B
ATOM	4245	CB	SER	B	181	23.615	8.457	22.774	1.00	28.11	B
ATOM	4246	CG	SER	B	181	22.674	9.033	23.654	1.00	30.74	B
ATOM	4247	C	SER	B	181	24.037	7.590	20.498	1.00	26.06	B
ATOM	4248	O	SER	B	181	24.182	6.370	20.554	1.00	25.12	B
ATOM	4249	N	MET	B	182	24.765	8.374	19.704	1.00	25.90	B
ATOM	4250	CA	MET	B	182	25.779	7.846	18.813	1.00	29.20	B
ATOM	4251	CB	MET	B	182	25.238	7.784	17.382	1.00	31.43	B
ATOM	4252	CG	MET	B	182	24.114	6.789	17.181	1.00	33.69	B
ATOM	4253	SD	MET	B	182	24.722	5.139	17.524	1.00	34.88	B
ATOM	4254	CE	MET	B	182	25.373	4.651	15.929	1.00	34.59	B
ATOM	4255	C	MET	B	182	27.001	8.758	18.834	1.00	30.52	B
ATOM	4256	O	MET	B	182	26.857	9.983	18.819	1.00	30.18	B
ATOM	4257	N	PRO	B	183	28.214	8.177	18.872	1.00	32.39	B
ATOM	4258	CD	PRO	B	183	28.529	6.737	18.860	1.00	34.00	B
ATOM	4259	CA	PRO	B	183	29.449	8.977	18.888	1.00	34.40	B
ATOM	4260	CB	PRO	B	183	30.521	7.940	19.199	1.00	34.66	B
ATOM	4261	CG	PRO	B	183	29.998	6.735	18.481	1.00	35.09	B
ATOM	4262	C	PRO	B	183	29.663	9.624	17.517	1.00	35.33	B
ATOM	4263	O	PRO	B	183	29.355	9.015	16.502	1.00	35.46	B
ATOM	4264	N	ILE	B	184	30.199	10.843	17.506	1.00	36.88	B
ATOM	4265	CA	ILE	B	184	30.445	11.589	16.271	1.00	38.38	B

Figure 1 (continued 43)

ATOM	4266	CB	ILE	B	184	29.676	12.942	16.305	1.00	37.59	B
ATOM	4267	CG2	ILE	B	184	30.131	13.872	15.192	1.00	39.18	B
ATOM	4268	CG1	ILE	B	184	28.185	12.670	16.154	1.00	39.46	B
ATOM	4269	CD1	ILE	B	184	27.857	11.818	14.939	1.00	38.79	B
ATOM	4270	C	ILE	B	184	31.926	11.864	15.976	1.00	39.26	B
ATOM	4271	O	ILE	B	184	32.266	12.371	14.913	1.00	39.33	B
ATOM	4272	N	GLY	B	185	32.810	11.528	16.906	1.00	40.53	B
ATOM	4273	CA	GLY	B	185	34.225	11.777	16.671	1.00	42.10	B
ATOM	4274	C	GLY	B	185	34.630	13.227	16.897	1.00	43.16	B
ATOM	4275	O	GLN	B	186	35.821	13.542	16.982	1.00	44.33	B
ATOM	4276	N	GLN	B	186	33.646	14.117	16.988	1.00	43.84	B
ATOM	4277	CA	GLN	B	186	33.898	15.541	17.208	1.00	44.08	B
ATOM	4278	CB	GLN	B	186	33.069	16.406	16.254	1.00	43.89	B
ATOM	4279	CG	GLN	B	186	33.456	16.388	14.800	1.00	44.39	B
ATOM	4280	CD	GLN	B	186	32.677	17.426	14.006	1.00	44.45	B
ATOM	4281	OE1	GLN	B	186	32.773	18.631	14.269	1.00	42.44	B
ATOM	4282	NE2	GLN	B	186	31.893	16.963	13.039	1.00	44.05	B
ATOM	4283	C	GLN	B	186	33.503	15.952	18.614	1.00	44.15	B
ATOM	4284	N	SER	B	187	32.650	15.325	19.228	1.00	43.83	B
ATOM	4285	CA	SER	B	187	34.115	17.019	19.115	1.00	43.99	B
ATOM	4286	CB	SER	B	187	33.779	17.544	20.434	1.00	44.53	B
ATOM	4287	CG	SER	B	187	35.025	18.105	21.138	1.00	45.53	B
ATOM	4288	O	SER	B	187	36.033	17.117	21.304	1.00	43.54	B
ATOM	4289	C	SER	B	187	32.797	18.675	20.121	1.00	43.42	B
ATOM	4290	O	LEU	B	188	33.117	19.573	19.338	1.00	42.54	B
ATOM	4291	N	LEU	B	188	31.603	18.635	20.705	1.00	41.93	B
ATOM	4292	CA	LEU	B	188	30.616	19.669	20.425	1.00	42.36	B
ATOM	4293	CB	LEU	B	188	29.425	19.083	19.652	1.00	42.40	B
ATOM	4294	CG	LEU	B	188	29.558	18.823	18.148	1.00	42.81	B
ATOM	4295	CD1	LEU	B	188	30.321	19.973	17.494	1.00	42.43	B
ATOM	4296	CD2	LEU	B	188	30.269	17.515	17.910	1.00	41.46	B
ATOM	4297	C	LEU	B	188	30.074	20.411	21.623	1.00	42.28	B
ATOM	4298	O	PRO	B	189	30.097	19.910	22.742	1.00	40.92	B
ATOM	4299	N	PRO	B	189	29.580	21.638	21.398	1.00	40.91	B
ATOM	4300	CD	PRO	B	189	29.691	22.410	20.147	1.00	39.91	B
ATOM	4301	CA	PRO	B	189	29.009	22.457	22.466	1.00	40.82	B
ATOM	4302	CB	PRO	B	189	28.784	23.810	21.793	1.00	41.55	B
ATOM	4303	CG	PRO	B	189	29.770	23.819	20.656	1.00	39.55	B
ATOM	4304	C	PRO	B	189	27.683	21.801	22.853	1.00	37.81	B
ATOM	4305	O	PRO	B	189	26.834	21.544	21.995	1.00	38.79	B
ATOM	4306	N	SER	B	190	27.507	21.512	24.134	1.00	38.03	B
ATOM	4307	CA	SER	B	190	26.266	20.889	24.577	1.00	38.64	B
ATOM	4308	CB	SER	B	190	26.237	20.860	26.103	1.00	41.63	B
ATOM	4309	CG	SER	B	190	27.459	20.337	26.593	1.00	36.48	B
ATOM	4310	C	SER	B	190	25.126	21.733	24.005	1.00	37.47	B
ATOM	4311	O	HIS	B	191	25.072	22.937	24.221	1.00	34.74	B
ATOM	4312	N	HIS	B	191	24.214	21.102	23.268	1.00	32.42	B
ATOM	4313	CA	HIS	B	191	23.122	21.831	22.620	1.00	33.72	B
ATOM	4314	CB	HIS	B	191	23.568	22.172	21.214	1.00	34.73	B
ATOM	4315	CG	HIS	B	191	23.168	23.535	20.772	1.00	35.24	B
ATOM	4316	CD2	HIS	B	191	22.084	23.968	20.094	1.00	35.16	B
ATOM	4317	ND1	HIS	B	191	23.936	24.649	21.031	1.00	36.06	B
ATOM	4318	CE1	HIS	B	191	23.339	25.714	20.527	1.00	35.42	B
ATOM	4319	NE2	HIS	B	191	22.212	25.328	19.955	1.00	31.38	B
ATOM	4320	C	HIS	B	191	21.803	21.029	22.537	1.00	29.69	B
ATOM	4321	O	SER	B	192	21.851	19.831	22.375	1.00	28.86	B
ATOM	4322	N	SER	B	192	20.649	21.695	22.605	1.00	28.56	B
ATOM	4323	CA	SER	B	192	19.354	20.993	22.547	1.00	32.04	B
ATOM	4324	CB	SER	B	192	18.819	20.691	23.955	1.00	28.26	B
ATOM	4325	CG	SER	B	192	19.649	19.762	24.617	1.00	29.68	B
ATOM	4326	C	SER	B	192	18.239	21.687	21.801	1.00	23.60	B
ATOM	4327	O	VAL	B	193	17.764	22.768	22.223	1.00	22.38	B
ATOM	4328	N	VAL	B	193	17.765	21.042	20.731	1.00	20.07	B
ATOM	4329	CA	VAL	B	193	16.676	21.602	19.942	1.00	22.51	B
ATOM	4330	CB	VAL	B	193	17.198	22.242	18.651	1.00	21.46	B
ATOM	4331	CG1	VAL	B	193	18.139	23.408	18.996	1.00	21.51	B
ATOM	4332	CG2	VAL	B	193	17.914	21.209	17.824	1.00	20.75	B
ATOM	4333	C	VAL	B	193	15.618	20.598	19.542	1.00	19.19	B
ATOM	4334	O	ILE	B	194	15.877	19.389	19.444	1.00	18.69	B
ATOM	4335	N	ILE	B	194	14.431	21.113	19.297	1.00	20.65	B
ATOM	4336	CA	ILE	B	194	13.300	20.279	18.885	1.00	20.91	B
ATOM	4337	CB	ILE	B	194	12.047	20.662	19.661	1.00	22.06	B
ATOM	4338	CG2	ILE	B	194	10.879	19.737	19.263	1.00	25.62	B
ATOM	4339	CG1	ILE	B	194	12.351	20.584	21.156	1.00	17.66	B
ATOM	4340	CD1	ILE	B	194	11.268	21.174	21.991	1.00	17.42	B
ATOM	4341	C	ILE	B	194	13.025	20.452	17.392	1.00	15.23	B
ATOM	4342	O	ILE	B	194	12.699	21.535	16.925	1.00	17.30	B
ATOM	4343	N	VAL	B	195	13.147	19.361	16.641	1.00	16.64	B
ATOM	4344	CA	VAL	B	195	12.878	19.360	15.212	1.00	16.68	B
ATOM	4345	CB	VAL	B	195	13.834	18.401	14.473	1.00	16.31	B
ATOM	4346	CG1	VAL	B	195	13.491	18.338	12.979	1.00	16.90	B
ATOM	4347	CG2	VAL	B	195	15.268	18.857	14.695	1.00	17.47	B
ATOM	4348	C	VAL	B	195	11.412	18.916	15.005	1.00	18.83	B
ATOM	4349	O	PRO	B	196	10.978	17.903	15.567	1.00	19.05	B
ATOM	4350	N	PRO	B	196	10.632	19.670	14.207	1.00	20.57	B
ATOM	4351	CD	PRO	B	196	8.772	19.364	13.933	1.00	22.10	B
ATOM	4352	CA	PRO	B	196	9.215	20.478	12.980	1.00	19.72	B
ATOM	4353	CB	PRO	B	196	9.793	21.504	13.114	1.00	18.66	B
ATOM	4354	CG	PRO	B	196	9.046	18.009	13.265	1.00	20.21	B
ATOM	4355	O	PRO	B	196	9.944	17.513	12.607	1.00	21.19	B
ATOM	4356	N	ARG	B	197	7.852	17.440	13.430	1.00	25.71	B
ATOM	4357	CA	ARG	B	197	7.519	16.149	12.846	1.00	30.00	B
ATOM	4358	CB	ARG	B	197	6.012	15.904	13.000	1.00	32.19	B
ATOM	4359	CG	ARG	B	197	5.519	14.646	12.322	1.00	35.51	B
ATOM	4360	CD	ARG	B	197	3.984	14.652	12.252	1.00	36.04	B
ATOM	4361	NE	ARG	B	197	3.458	15.525	11.200	1.00	36.85	B
ATOM	4362	CZ	ARG	B	197	3.290	15.155	9.929	1.00	37.72	B
ATOM	4363	NH1	ARG	B	197	3.606	13.925	9.536	1.00		B
ATOM	4365	NH2	ARG	B	197	2.793	16.012	9.051	1.00		B

Figure 1 (continued 44)

ATOM	4366	C	ARG	B	197	7.873	16.032	11.374	1.00	20.20
ATOM	4367	O	ARG	B	197	8.529	15.075	10.978	1.00	18.75
ATOM	4368	N	LYS	B	198	7.426	16.982	10.553	1.00	19.22
ATOM	4369	CA	LYS	B	198	7.713	16.900	9.122	1.00	20.05
ATOM	4370	CB	LYS	B	198	6.956	17.965	8.323	1.00	22.68
ATOM	4371	CG	LYS	B	198	5.458	17.685	8.160	1.00	27.88
ATOM	4372	CD	LYS	B	198	4.815	18.821	7.335	1.00	32.73
ATOM	4373	CE	LYS	B	198	3.313	18.648	7.098	1.00	36.66
ATOM	4374	NZ	LYS	B	198	2.468	18.767	8.340	1.00	38.58
ATOM	4375	C	LYS	B	198	9.190	17.058	8.872	1.00	17.68
ATOM	4376	O	LYS	B	198	9.709	16.583	7.873	1.00	19.10
ATOM	4377	N	GLY	B	199	9.866	17.731	9.790	1.00	15.43
ATOM	4378	CA	GLY	B	199	11.292	17.946	9.628	1.00	16.07
ATOM	4379	CB	GLY	B	199	12.045	16.641	9.766	1.00	15.66
ATOM	4380	O	GLY	B	199	13.015	16.380	9.059	1.00	15.20
ATOM	4381	N	VAL	B	200	11.624	15.841	10.737	1.00	14.98
ATOM	4382	CA	VAL	B	200	12.245	14.548	10.958	1.00	15.69
ATOM	4383	CB	VAL	B	200	11.617	13.864	12.175	1.00	16.41
ATOM	4384	CG1	VAL	B	200	12.217	12.449	12.354	1.00	18.05
ATOM	4385	CG2	VAL	B	200	11.899	14.718	13.380	1.00	17.11
ATOM	4386	C	VAL	B	200	12.056	13.678	9.722	1.00	15.55
ATOM	4387	O	VAL	B	200	12.977	12.967	9.284	1.00	17.07
ATOM	4388	N	ILE	B	201	10.858	13.703	9.165	1.00	18.07
ATOM	4389	CA	ILE	B	201	10.567	12.942	7.950	1.00	18.45
ATOM	4390	CB	ILE	B	201	9.084	13.098	7.563	1.00	19.51
ATOM	4391	CG	ILE	B	201	8.814	12.494	6.175	1.00	21.46
ATOM	4392	CG1	ILE	B	201	8.238	12.391	8.602	1.00	20.58
ATOM	4393	CD1	ILE	B	201	6.738	12.554	8.392	1.00	24.22
ATOM	4394	C	ILE	B	201	11.447	13.367	6.789	1.00	18.72
ATOM	4395	O	ILE	B	201	11.960	12.519	6.065	1.00	20.22
ATOM	4396	N	GLU	B	202	11.643	14.673	6.607	1.00	19.15
ATOM	4397	CA	GLU	B	202	12.483	15.152	5.514	1.00	20.05
ATOM	4398	CB	GLU	B	202	12.426	16.681	5.362	1.00	21.56
ATOM	4399	CG	GLU	B	202	11.174	17.168	4.689	1.00	24.74
ATOM	4400	CD	GLU	B	202	10.866	16.349	3.452	1.00	27.41
ATOM	4401	OE1	GLU	B	202	9.725	15.850	3.346	1.00	27.85
ATOM	4402	OE2	GLU	B	202	11.770	16.185	2.602	1.00	28.02
ATOM	4403	C	GLU	B	202	13.923	14.751	5.734	1.00	20.02
ATOM	4404	O	GLU	B	202	14.602	14.397	4.773	1.00	21.05
ATOM	4405	N	LEU	B	203	14.405	14.838	6.979	1.00	18.48
ATOM	4406	CA	LEU	B	203	15.780	14.445	7.272	1.00	19.51
ATOM	4407	CB	LEU	B	203	16.102	14.570	8.764	1.00	20.96
ATOM	4408	CG	LEU	B	203	16.378	15.983	9.271	1.00	22.79
ATOM	4409	CD1	LEU	B	203	16.571	15.960	10.797	1.00	23.58
ATOM	4410	CD2	LEU	B	203	17.644	16.526	8.566	1.00	24.88
ATOM	4411	C	LEU	B	203	15.987	13.009	6.848	1.00	20.44
ATOM	4412	O	LEU	B	203	17.008	12.674	6.231	1.00	18.72
ATOM	4413	N	MET	B	204	15.027	12.142	7.171	1.00	18.16
ATOM	4414	CA	MET	B	204	15.153	10.734	6.784	1.00	21.15
ATOM	4415	CB	MET	B	204	14.008	9.914	7.399	1.00	23.53
ATOM	4416	CG	MET	B	204	13.959	8.461	6.938	1.00	29.56
ATOM	4417	SD	MET	B	204	15.384	7.475	7.480	1.00	38.65
ATOM	4418	CE	MET	B	204	15.782	8.308	8.992	1.00	30.14
ATOM	4419	C	MET	B	204	15.147	10.530	5.265	1.00	22.14
ATOM	4420	O	MET	B	204	15.920	9.728	4.732	1.00	22.11
ATOM	4421	N	ARG	B	205	14.278	11.264	4.579	1.00	22.90
ATOM	4422	CA	ARG	B	205	14.147	11.174	3.132	1.00	25.90
ATOM	4423	CB	ARG	B	205	13.008	12.052	2.631	1.00	28.24
ATOM	4424	CG	ARG	B	205	11.659	11.451	2.747	1.00	31.40
ATOM	4425	CD	ARG	B	205	10.612	12.462	2.312	1.00	33.52
ATOM	4426	NE	ARG	B	205	9.282	11.913	2.527	1.00	34.98
ATOM	4427	CZ	ARG	B	205	8.155	12.614	2.484	1.00	36.39
ATOM	4428	NH1	ARG	B	205	8.186	13.912	2.228	1.00	36.54
ATOM	4429	NH2	ARG	B	205	6.997	12.008	2.717	1.00	36.70
ATOM	4430	C	ARG	B	205	15.360	11.583	2.355	1.00	26.12
ATOM	4431	O	ARG	B	205	15.548	11.131	1.226	1.00	25.57
ATOM	4432	N	MET	B	206	16.182	12.453	2.923	1.00	25.37
ATOM	4433	CA	MET	B	206	17.332	12.907	2.167	1.00	26.52
ATOM	4434	CB	MET	B	206	17.690	14.334	2.563	1.00	27.58
ATOM	4435	CG	MET	B	206	18.358	14.497	3.881	1.00	25.49
ATOM	4436	SD	MET	B	206	18.341	16.237	4.294	1.00	27.01
ATOM	4437	CE	MET	B	206	18.905	16.967	2.700	1.00	25.57
ATOM	4438	C	MET	B	206	18.541	12.008	2.269	1.00	27.45
ATOM	4439	O	MET	B	206	19.584	12.282	1.669	1.00	26.91
ATOM	4440	N	LEU	B	207	18.407	10.934	3.036	1.00	28.07
ATOM	4441	CA	LEU	B	207	19.512	10.010	3.172	1.00	30.58
ATOM	4442	CB	LEU	B	207	19.407	9.290	4.512	1.00	29.11
ATOM	4443	CG	LEU	B	207	19.312	10.219	5.724	1.00	26.96
ATOM	4444	CD1	LEU	B	207	19.271	9.343	6.995	1.00	27.09
ATOM	4445	CD2	LEU	B	207	20.482	11.190	5.763	1.00	24.96
ATOM	4446	C	LEU	B	207	19.442	9.029	2.000	1.00	33.44
ATOM	4447	O	LEU	B	207	18.468	8.306	1.835	1.00	34.23
ATOM	4448	N	ASP	B	208	20.476	9.020	1.170	1.00	37.29
ATOM	4449	CA	ASP	B	208	20.490	8.136	0.016	1.00	40.97
ATOM	4450	CB	ASP	B	208	21.349	8.726	-1.099	1.00	42.41
ATOM	4451	CG	ASP	B	208	22.832	8.627	-0.799	1.00	43.64
ATOM	4452	OD1	ASP	B	208	23.355	9.451	-0.024	1.00	45.03
ATOM	4453	OD2	ASP	B	208	23.483	7.705	-1.330	1.00	46.54
ATOM	4454	C	ASP	B	208	21.079	6.806	0.437	1.00	42.45
ATOM	4455	O	ASP	B	208	20.948	5.805	-0.266	1.00	44.07
ATOM	4456	N	GLY	B	209	21.728	6.795	1.593	1.00	43.63
ATOM	4457	CA	GLY	B	209	22.347	5.573	2.055	1.00	45.09
ATOM	4458	C	GLY	B	209	23.590	5.341	1.220	1.00	45.45
ATOM	4459	O	GLY	B	209	23.921	4.207	0.865	1.00	46.37
ATOM	4460	N	GLY	B	210	24.273	6.434	0.892	1.00	45.49
ATOM	4461	CA	GLY	B	210	25.489	6.350	0.111	1.00	44.86
ATOM	4462	C	GLY	B	210	26.648	6.835	0.952	1.00	44.61
ATOM	4463	O	GLY	B	210	26.506	7.031	2.158	1.00	44.29
ATOM	4464	N	ASP	B	211	27.793	7.036	0.311	1.00	44.84
ATOM	4465	CA	ASP	B	211	28.998	7.499	0.985	1.00	44.68

Figure 1 (continued 45)

ATOM	4466	CB	ASP	B	211	30.220	7.108	0.154	1.00	46.96	B
ATOM	4467	CG	ASP	B	211	30.015	7.377	-1.327	1.00	49.59	B
ATOM	4468	OD1	ASP	B	211	29.929	8.565	-1.718	1.00	51.33	B
ATOM	4469	OD2	ASP	B	211	29.924	6.398	-2.100	1.00	51.23	B
ATOM	4470	C	ASP	B	211	29.023	9.008	1.253	1.00	43.00	B
ATOM	4471	O	ASN	B	212	29.901	9.493	1.970	1.00	42.86	B
ATOM	4472	N	ASN	B	212	28.082	9.758	0.679	1.00	40.95	B
ATOM	4473	CA	ASN	B	212	28.054	11.201	0.917	1.00	38.13	B
ATOM	4474	CB	ASN	B	212	26.875	11.872	0.200	1.00	40.65	B
ATOM	4475	CG	ASN	B	212	26.909	11.679	-1.298	1.00	42.99	B
ATOM	4476	OD1	ASN	B	212	26.795	10.553	-1.799	1.00	46.74	B
ATOM	4477	ND2	ASN	B	212	27.064	12.774	-2.026	1.00	43.95	B
ATOM	4478	C	ASN	B	212	27.891	11.442	2.417	1.00	35.10	B
ATOM	4479	O	ASN	B	212	27.031	10.845	3.062	1.00	34.26	B
ATOM	4480	N	PRO	B	213	28.722	12.313	2.992	1.00	33.01	B
ATOM	4481	CD	PRO	B	213	29.862	13.029	2.379	1.00	29.13	B
ATOM	4482	CA	PRO	B	213	28.622	12.604	4.422	1.00	31.02	B
ATOM	4483	CB	PRO	B	213	29.993	13.183	4.742	1.00	31.64	B
ATOM	4484	CG	PRO	B	213	30.301	13.958	3.492	1.00	26.76	B
ATOM	4485	C	PRO	B	213	27.493	13.627	4.641	1.00	25.59	B
ATOM	4486	O	PRO	B	213	27.099	14.330	3.711	1.00	23.19	B
ATOM	4487	N	LEU	B	214	26.964	13.676	5.856	1.00	22.69	B
ATOM	4488	CA	LEU	B	214	25.892	14.608	6.189	1.00	25.15	B
ATOM	4489	CB	LEU	B	214	24.805	13.875	7.006	1.00	27.21	B
ATOM	4490	CG	LEU	B	214	23.706	14.726	7.624	1.00	28.20	B
ATOM	4491	CD1	LEU	B	214	22.868	15.298	6.520	1.00	27.67	B
ATOM	4492	CD2	LEU	B	214	22.840	13.877	8.557	1.00	21.63	B
ATOM	4493	C	LEU	B	214	26.465	15.766	6.993	1.00	22.98	B
ATOM	4494	O	LEU	B	214	27.109	15.551	8.008	1.00	20.26	B
ATOM	4495	N	ARG	B	215	26.255	17.004	6.540	1.00	20.31	B
ATOM	4496	CA	ARG	B	215	26.763	18.148	7.275	1.00	24.44	B
ATOM	4497	CB	ARG	B	215	27.529	19.121	6.367	1.00	28.96	B
ATOM	4498	CG	ARG	B	215	28.163	20.269	7.151	1.00	34.52	B
ATOM	4499	CD	ARG	B	215	29.021	21.199	6.288	1.00	38.13	B
ATOM	4500	NE	ARG	B	215	28.826	22.593	6.691	1.00	39.89	B
ATOM	4501	CZ	ARG	B	215	28.386	23.555	5.879	1.00	41.19	B
ATOM	4502	NH1	ARG	B	215	28.100	23.297	4.605	1.00	42.36	B
ATOM	4503	NH2	ARG	B	215	28.197	24.775	7.923	1.00	19.25	B
ATOM	4504	C	ARG	B	215	25.607	18.863	6.352	1.00	19.32	B
ATOM	4505	O	ARG	B	215	24.672	19.274	7.253	1.00	16.59	B
ATOM	4506	N	VAL	B	216	25.702	19.027	9.231	1.00	16.36	B
ATOM	4507	CA	VAL	B	216	24.645	19.655	10.002	1.00	15.73	B
ATOM	4508	CB	VAL	B	216	24.224	18.737	11.177	1.00	16.54	B
ATOM	4509	CG1	VAL	B	216	23.045	19.383	11.949	1.00	16.55	B
ATOM	4510	CG2	VAL	B	216	23.924	17.379	10.674	1.00	18.40	B
ATOM	4511	C	VAL	B	216	25.029	20.994	10.583	1.00	18.97	B
ATOM	4512	O	VAL	B	216	26.137	21.168	11.094	1.00	16.54	B
ATOM	4513	N	GLN	B	217	24.104	21.951	10.521	1.00	18.52	B
ATOM	4514	CA	GLN	B	217	24.331	23.265	11.096	1.00	19.71	B
ATOM	4515	CB	GLN	B	217	24.482	24.346	10.021	1.00	21.74	B
ATOM	4516	CG	GLN	B	217	25.754	24.294	9.206	1.00	24.98	B
ATOM	4517	CD	GLN	B	217	25.778	25.415	8.168	1.00	28.72	B
ATOM	4518	OE1	GLN	B	217	26.529	26.403	8.299	1.00	23.49	B
ATOM	4519	NE2	GLN	B	217	24.932	25.283	7.141	1.00	18.28	B
ATOM	4520	C	GLN	B	217	23.088	23.566	11.929	1.00	17.82	B
ATOM	4521	O	GLN	B	217	21.970	23.360	11.466	1.00	17.89	B
ATOM	4522	N	ILE	B	218	23.293	23.999	13.170	1.00	18.52	B
ATOM	4523	CA	ILE	B	218	22.184	24.327	14.049	1.00	19.36	B
ATOM	4524	CB	ILE	B	218	22.125	23.382	15.290	1.00	21.63	B
ATOM	4525	CG2	ILE	B	218	20.877	23.687	16.133	1.00	19.91	B
ATOM	4526	CG1	ILE	B	218	22.098	21.932	14.849	1.00	19.55	B
ATOM	4527	CD1	ILE	B	218	22.008	20.959	16.021	1.00	19.93	B
ATOM	4528	C	ILE	B	218	22.333	25.745	14.567	1.00	18.55	B
ATOM	4529	O	ILE	B	218	23.418	26.145	15.038	1.00	18.45	B
ATOM	4530	N	GLY	B	219	21.231	26.488	14.485	1.00	20.72	B
ATOM	4531	CA	GLY	B	219	21.173	27.845	14.966	1.00	21.48	B
ATOM	4532	C	GLY	B	219	20.213	27.895	16.139	1.00	20.11	B
ATOM	4533	O	GLY	B	219	19.724	26.859	16.621	1.00	23.01	B
ATOM	4534	N	SER	B	220	19.917	29.104	16.597	1.00	23.61	B
ATOM	4535	CA	SER	B	220	19.014	29.266	17.724	1.00	26.05	B
ATOM	4536	CB	SER	B	220	19.009	30.718	18.199	1.00	29.78	B
ATOM	4537	CG	SER	B	220	18.517	31.556	17.166	1.00	23.25	B
ATOM	4538	C	SER	B	220	17.593	28.866	17.345	1.00	21.92	B
ATOM	4539	O	SER	B	220	16.825	28.449	18.203	1.00	21.87	B
ATOM	4540	N	ASN	B	221	17.240	28.989	16.068	1.00	21.62	B
ATOM	4541	CA	ASN	B	221	15.879	28.662	15.667	1.00	25.88	B
ATOM	4542	CB	ASN	B	221	15.065	29.948	15.549	1.00	30.93	B
ATOM	4543	CG	ASN	B	221	15.037	30.730	16.850	1.00	35.31	B
ATOM	4544	OD1	ASN	B	221	15.890	31.585	17.095	1.00	32.95	B
ATOM	4545	ND2	ASN	B	221	14.067	30.423	17.700	1.00	18.27	B
ATOM	4546	C	ASN	B	221	15.750	27.880	14.378	1.00	18.70	B
ATOM	4547	O	ASN	B	221	14.657	27.787	13.830	1.00	18.16	B
ATOM	4548	N	ASN	B	222	16.844	27.284	13.919	1.00	16.52	B
ATOM	4549	CA	ASN	B	222	16.822	26.555	12.653	1.00	19.66	B
ATOM	4550	CB	ASN	B	222	17.258	27.445	11.472	1.00	21.30	B
ATOM	4551	CG	ASN	B	222	16.359	28.636	11.258	1.00	23.15	B
ATOM	4552	OD1	ASN	B	222	16.377	29.589	12.038	1.00	22.47	B
ATOM	4553	ND2	ASN	B	222	15.570	28.607	10.172	1.00	15.05	B
ATOM	4554	C	ASN	B	222	17.820	25.447	12.674	1.00	15.87	B
ATOM	4555	O	ASN	B	222	18.762	25.461	13.464	1.00	14.78	B
ATOM	4556	N	ILE	B	223	17.571	24.457	11.836	1.00	13.60	B
ATOM	4557	CA	ILE	B	223	18.531	23.373	11.657	1.00	13.56	B
ATOM	4558	CB	ILE	B	223	18.077	22.036	12.294	1.00	14.77	B
ATOM	4559	CG2	ILE	B	223	16.722	21.592	11.714	1.00	15.05	B
ATOM	4560	CG1	ILE	B	223	19.172	20.962	12.069	1.00	17.92	B
ATOM	4561	CD1	ILE	B	223	18.996	19.763	13.023	1.00	15.44	B
ATOM	4562	C	ILE	B	223	18.638	23.212	10.158	1.00	15.61	B
ATOM	4563	O	ILE	B	223	17.641	23.372	9.433	1.00	15.47	B
ATOM	4564	N	ARG	B	224	19.860	22.950	9.685	1.00	14.89	B
ATOM	4565	CA	ARG	B	224	20.103	22.744	8.267	1.00		B

Figure 1 (continued 46)

[illegible]

Figure 1 (continued 47)

ATOM	4666	CD2	LEU	B	236	15.474	22.974	15.228	1.00	16.38
ATOM	4667	C	LEU	B	236	11.594	24.879	15.982	1.00	18.39
ATOM	4668	O	LEU	B	236	10.986	25.947	15.802	1.00	19.38
ATOM	4669	N	VAL	B	237	11.185	23.941	16.831	1.00	21.05
ATOM	4670	CA	VAL	B	237	9.983	24.091	17.638	1.00	23.90
ATOM	4671	CB	VAL	B	237	9.278	22.707	17.848	1.00	24.44
ATOM	4672	CG1	VAL	B	237	8.085	22.831	18.837	1.00	25.05
ATOM	4673	CG2	VAL	B	237	8.774	22.189	16.503	1.00	26.22
ATOM	4674	C	VAL	B	237	10.380	24.655	19.000	1.00	26.41
ATOM	4675	O	VAL	B	237	11.366	24.235	19.589	1.00	25.35
ATOM	4676	N	ASP	B	238	9.639	25.636	19.496	1.00	32.01
ATOM	4677	CA	ASP	B	238	9.975	26.158	20.816	1.00	37.53
ATOM	4678	CB	ASP	B	238	9.528	27.603	20.977	1.00	40.37
ATOM	4679	CG	ASP	B	238	10.234	28.530	20.022	1.00	42.20
ATOM	4680	OD1	ASP	B	238	11.453	28.325	19.791	1.00	43.09
ATOM	4681	OD2	ASP	B	238	9.571	29.466	19.514	1.00	45.01
ATOM	4682	C	ASP	B	238	9.284	25.302	21.852	1.00	39.40
ATOM	4683	O	ASP	B	238	8.449	24.457	21.519	1.00	41.81
ATOM	4684	N	GLY	B	239	9.638	25.498	23.111	1.00	41.31
ATOM	4685	CA	GLY	B	239	9.004	24.722	24.157	1.00	42.54
ATOM	4686	C	GLY	B	239	10.019	24.022	25.019	1.00	43.17
ATOM	4687	O	GLY	B	239	11.188	23.944	24.665	1.00	42.73
ATOM	4688	N	ARG	B	240	9.572	23.506	26.156	1.00	44.77
ATOM	4689	CA	ARG	B	240	10.473	22.812	27.062	1.00	45.41
ATOM	4690	CB	ARG	B	240	10.215	23.260	28.497	1.00	47.67
ATOM	4691	CG	ARG	B	240	8.807	22.985	28.997	1.00	50.38
ATOM	4692	CD	ARG	B	240	8.662	23.521	30.408	1.00	52.39
ATOM	4693	NE	ARG	B	240	8.988	24.942	30.464	1.00	53.18
ATOM	4694	CZ	ARG	B	240	9.345	25.580	31.572	1.00	54.35
ATOM	4695	NH1	ARG	B	240	9.422	24.925	32.727	1.00	53.83
ATOM	4696	NH2	ARG	B	240	9.638	26.871	31.517	1.00	55.03
ATOM	4697	C	ARG	B	240	10.277	21.306	26.942	1.00	44.25
ATOM	4698	O	ARG	B	240	9.199	20.790	27.237	1.00	45.09
ATOM	4699	N	PHE	B	241	11.331	20.615	26.520	1.00	42.31
ATOM	4700	CA	PHE	B	241	11.290	19.167	26.326	1.00	40.40
ATOM	4701	CB	PHE	B	241	12.024	18.818	25.019	1.00	37.04
ATOM	4702	CG	PHE	B	241	11.584	17.518	24.380	1.00	33.05
ATOM	4703	CD1	PHE	B	241	12.109	16.303	24.798	1.00	32.26
ATOM	4704	CD2	PHE	B	241	10.666	17.529	23.338	1.00	30.96
ATOM	4705	CE1	PHE	B	241	11.727	15.108	24.179	1.00	29.39
ATOM	4706	CE2	PHE	B	241	10.276	16.347	22.714	1.00	29.62
ATOM	4707	CZ	PHE	B	241	10.814	15.134	23.141	1.00	28.51
ATOM	4708	C	PHE	B	241	11.892	18.398	27.511	1.00	39.78
ATOM	4709	O	PHE	B	241	12.919	18.785	28.077	1.00	40.91
ATOM	4710	N	PRO	B	242	11.254	17.279	27.890	1.00	38.82
ATOM	4711	CD	PRO	B	242	9.987	16.826	27.286	1.00	37.70
ATOM	4712	CA	PRO	B	242	11.660	16.404	28.997	1.00	37.16
ATOM	4713	CB	PRO	B	242	10.688	15.230	28.874	1.00	37.98
ATOM	4714	CG	PRO	B	242	9.448	15.869	28.336	1.00	37.43
ATOM	4715	C	PRO	B	242	13.124	15.947	28.987	1.00	36.91
ATOM	4716	O	PRO	B	242	13.728	15.748	27.925	1.00	35.36
ATOM	4717	N	ASP	B	243	13.675	15.763	30.184	1.00	35.76
ATOM	4718	CA	ASP	B	243	15.053	15.323	30.369	1.00	36.57
ATOM	4719	CB	ASP	B	243	15.625	15.957	31.639	1.00	35.26
ATOM	4720	CG	ASP	B	243	17.064	15.549	31.907	1.00	36.71
ATOM	4721	OD1	ASP	B	243	17.556	14.587	31.281	1.00	36.01
ATOM	4722	OD2	ASP	B	243	17.709	16.188	32.767	1.00	36.91
ATOM	4723	C	ASP	B	243	15.114	13.796	30.495	1.00	36.45
ATOM	4724	O	ASP	B	243	14.919	13.251	31.576	1.00	36.71
ATOM	4725	N	TYR	B	244	15.419	13.103	29.407	1.00	36.69
ATOM	4726	CA	TYR	B	244	15.477	12.638	29.446	1.00	36.02
ATOM	4727	CB	TYR	B	244	16.148	11.089	28.186	1.00	34.53
ATOM	4728	CG	TYR	B	244	17.657	10.998	28.255	1.00	34.00
ATOM	4729	CD1	TYR	B	244	18.462	12.105	27.968	1.00	32.87
ATOM	4730	CE1	TYR	B	244	19.858	12.000	27.984	1.00	34.13
ATOM	4731	CD2	TYR	B	244	18.281	9.791	28.566	1.00	33.14
ATOM	4732	CE2	TYR	B	244	19.665	9.672	28.581	1.00	34.72
ATOM	4733	CZ	TYR	B	244	20.449	10.783	28.283	1.00	34.56
ATOM	4734	OH	TYR	B	244	21.811	10.638	28.235	1.00	36.14
ATOM	4735	C	TYR	B	244	16.199	11.060	30.673	1.00	37.56
ATOM	4736	O	TYR	B	244	15.795	10.029	31.215	1.00	36.17
ATOM	4737	N	ARG	B	245	17.269	11.728	31.092	1.00	40.14
ATOM	4738	CA	ARG	B	245	18.074	11.296	32.231	1.00	40.81
ATOM	4739	CB	ARG	B	245	19.166	12.333	32.518	1.00	43.08
ATOM	4740	CG	ARG	B	245	20.029	12.665	31.319	1.00	43.61
ATOM	4741	CD	ARG	B	245	21.075	13.731	31.631	1.00	45.10
ATOM	4742	NE	ARG	B	245	21.787	14.137	30.420	1.00	45.50
ATOM	4743	CZ	ARG	B	245	21.231	14.807	29.413	1.00	44.89
ATOM	4744	NH1	ARG	B	245	19.952	15.157	29.464	1.00	46.19
ATOM	4745	NH2	ARG	B	245	21.956	15.131	28.348	1.00	40.09
ATOM	4746	C	ARG	B	245	17.233	11.102	33.486	1.00	40.05
ATOM	4747	O	ARG	B	245	17.574	10.297	34.352	1.00	39.85
ATOM	4748	N	ARG	B	246	16.133	11.840	34.707	1.00	40.96
ATOM	4749	CA	ARG	B	246	15.239	11.808	34.984	1.00	43.17
ATOM	4750	CB	ARG	B	246	14.755	13.227	35.113	1.00	46.06
ATOM	4751	CG	ARG	B	246	15.880	14.252	36.529	1.00	47.96
ATOM	4752	CD	ARG	B	246	16.443	14.295	37.524	1.00	49.96
ATOM	4753	NE	ARG	B	246	15.374	14.318	37.477	1.00	50.99
ATOM	4754	CZ	ARG	B	246	14.316	15.126	36.481	1.00	51.52
ATOM	4755	NH1	ARG	B	246	14.169	15.992	38.430	1.00	52.32
ATOM	4756	NH2	ARG	B	246	13.396	15.067	34.566	1.00	40.13
ATOM	4757	C	ARG	B	246	14.022	10.889	35.560	1.00	39.22
ATOM	4758	O	ARG	B	246	13.384	10.536	33.327	1.00	38.72
ATOM	4759	N	VAL	B	247	13.695	10.532	33.018	1.00	36.88
ATOM	4760	CA	VAL	B	247	12.553	9.675	31.585	1.00	37.39
ATOM	4761	CB	VAL	B	247	12.061	9.942	31.216	1.00	36.97
ATOM	4762	CG1	VAL	B	247	10.930	8.991	31.462	1.00	37.68
ATOM	4763	CG2	VAL	B	247	11.624	11.391	33.133	1.00	35.57
ATOM	4764	C	VAL	B	247	12.962	8.218	33.308	1.00	36.36
ATOM	4765	O	VAL	B	247	12.125	7.334			

Figure 1 (continued 48)

ATOM	4766	N	LEU	B	248	14.260	7.974	33.019	1.00	34.36
ATOM	4767	CA	LEU	B	248	14.797	6.627	33.124	1.00	34.03
ATOM	4768	CB	LEU	B	248	16.296	6.621	32.855	1.00	33.66
ATOM	4769	CG	LEU	B	248	16.785	7.109	31.499	1.00	33.85
ATOM	4770	CD1	LEU	B	248	18.285	6.813	31.398	1.00	34.48
ATOM	4771	CD2	LEU	B	248	16.017	6.403	30.386	1.00	33.89
ATOM	4772	C	LEU	B	248	14.564	6.083	34.525	1.00	34.01
ATOM	4773	O	LEU	B	248	14.860	6.756	35.519	1.00	32.99
ATOM	4774	N	PRO	B	249	14.038	4.851	34.622	1.00	33.37
ATOM	4775	CD	PRO	B	249	13.707	3.936	33.514	1.00	32.25
ATOM	4776	CA	PRO	B	249	13.776	4.221	35.921	1.00	33.57
ATOM	4777	CB	PRO	B	249	13.565	2.751	35.546	1.00	32.82
ATOM	4778	CG	PRO	B	249	12.921	2.845	34.210	1.00	32.30
ATOM	4779	C	PRO	B	249	14.965	4.423	36.875	1.00	33.81
ATOM	4780	O	PRO	B	249	16.113	4.182	36.514	1.00	31.74
ATOM	4781	N	LYS	B	250	14.672	4.869	38.091	1.00	36.30
ATOM	4782	CA	LYS	B	250	15.695	5.128	39.102	1.00	39.83
ATOM	4783	CB	LYS	B	250	15.024	5.653	40.370	1.00	41.65
ATOM	4784	CG	LYS	B	250	13.622	6.224	40.144	1.00	44.53
ATOM	4785	CD	LYS	B	250	12.980	6.637	41.466	1.00	46.40
ATOM	4786	CE	LYS	B	250	11.562	7.139	41.267	1.00	47.75
ATOM	4787	NZ	LYS	B	250	10.957	7.618	42.538	1.00	48.54
ATOM	4788	C	LYS	B	250	16.562	3.912	39.454	1.00	40.80
ATOM	4789	O	LYS	B	250	17.773	3.915	39.240	1.00	42.14
ATOM	4790	N	ASN	B	251	15.944	2.881	40.016	1.00	40.30
ATOM	4791	CA	ASN	B	251	16.687	1.686	40.388	1.00	41.84
ATOM	4792	CB	ASN	B	251	16.907	1.661	41.899	1.00	43.14
ATOM	4793	CG	ASN	B	251	17.875	2.734	42.365	1.00	44.47
ATOM	4794	OD1	ASN	B	251	17.623	3.421	43.353	1.00	45.51
ATOM	4795	ND2	ASN	B	251	18.996	2.873	41.662	1.00	45.61
ATOM	4796	C	ASN	B	251	15.976	0.413	39.942	1.00	41.06
ATOM	4797	O	ASN	B	251	15.388	-0.302	40.754	1.00	40.34
ATOM	4798	N	PRO	B	252	16.020	0.121	38.634	1.00	40.93
ATOM	4799	CA	PRO	B	252	16.646	0.951	37.592	1.00	40.87
ATOM	4800	CB	PRO	B	252	15.384	-1.069	38.051	1.00	40.56
ATOM	4801	CG	PRO	B	252	15.505	-0.839	36.539	1.00	40.95
ATOM	4802	C	PRO	B	252	15.797	-0.628	36.393	1.00	41.84
ATOM	4803	O	PRO	B	252	16.144	-2.323	38.481	1.00	40.59
ATOM	4804	N	ASP	B	253	16.811	-2.953	37.666	1.00	41.49
ATOM	4805	CA	ASP	B	253	16.024	-2.681	39.754	1.00	39.23
ATOM	4806	CB	ASP	B	253	16.725	-3.833	40.318	1.00	38.72
ATOM	4807	CG	ASP	B	253	16.316	-4.011	41.799	1.00	40.83
ATOM	4808	OD1	ASP	B	253	14.803	-4.237	41.995	1.00	42.90
ATOM	4809	OD2	ASP	B	253	13.992	-3.318	41.739	1.00	44.02
ATOM	4810	C	ASP	B	253	14.412	-5.347	42.423	1.00	44.75
ATOM	4811	O	ASP	B	253	16.616	-5.183	39.585	1.00	36.72
ATOM	4812	N	LYS	B	254	17.601	-5.922	39.478	1.00	36.03
ATOM	4813	CA	LYS	B	254	15.432	-5.484	39.066	1.00	32.67
ATOM	4814	CB	LYS	B	254	15.164	-6.751	38.403	1.00	30.08
ATOM	4815	CG	LYS	B	254	13.688	-7.106	38.593	1.00	28.89
ATOM	4816	CD	LYS	B	254	13.194	-7.092	40.049	1.00	29.78
ATOM	4817	CE	LYS	B	254	11.561	-7.160	40.098	1.00	28.23
ATOM	4818	NZ	LYS	B	254	11.120	-7.160	41.515	1.00	33.00
ATOM	4819	C	LYS	B	254	11.584	-5.968	42.297	1.00	33.49
ATOM	4820	O	LYS	B	254	15.489	-6.736	36.912	1.00	29.93
ATOM	4821	N	HIS	B	255	14.811	-6.060	36.135	1.00	30.36
ATOM	4822	CA	HIS	B	255	16.495	-7.501	36.519	1.00	27.24
ATOM	4823	CB	HIS	B	255	16.897	-7.564	35.118	1.00	26.91
ATOM	4824	CG	HIS	B	255	18.402	-7.339	34.966	1.00	30.35
ATOM	4825	CD2	HIS	B	255	18.876	-6.000	35.429	1.00	33.70
ATOM	4826	ND1	HIS	B	255	20.129	-5.522	35.617	1.00	34.19
ATOM	4827	CE1	HIS	B	255	18.021	-4.950	35.695	1.00	35.10
ATOM	4828	NE2	HIS	B	255	18.730	-3.882	36.025	1.00	35.55
ATOM	4829	C	HIS	B	255	20.011	-4.204	35.986	1.00	34.99
ATOM	4830	O	HIS	B	255	16.587	-8.885	34.453	1.00	24.52
ATOM	4831	N	LEU	B	256	16.979	-9.935	34.936	1.00	23.10
ATOM	4832	CA	LEU	B	256	15.923	-8.824	33.307	1.00	22.74
ATOM	4833	CB	LEU	B	256	15.606	-10.014	32.551	1.00	21.40
ATOM	4834	CG	LEU	B	256	14.080	-10.157	32.461	1.00	23.90
ATOM	4835	CD1	LEU	B	256	13.435	-11.154	31.508	1.00	24.90
ATOM	4836	CD2	LEU	B	256	12.064	-11.555	32.033	1.00	26.89
ATOM	4837	C	LEU	B	256	13.322	-10.514	30.136	1.00	23.55
ATOM	4838	O	LEU	B	256	16.210	-9.867	31.154	1.00	19.61
ATOM	4839	N	GLU	B	257	16.191	-8.768	30.581	1.00	18.29
ATOM	4840	CA	GLU	B	257	16.774	-10.955	30.641	1.00	18.37
ATOM	4841	CB	GLU	B	257	17.329	-10.973	29.287	1.00	18.54
ATOM	4842	CG	GLU	B	257	18.848	-11.229	29.318	1.00	21.51
ATOM	4843	CD	GLU	B	257	19.681	-10.093	29.921	1.00	27.65
ATOM	4844	OE1	GLU	B	257	19.758	-10.132	31.460	1.00	31.19
ATOM	4845	OE2	GLU	B	257	19.940	-11.236	32.023	1.00	33.27
ATOM	4846	C	GLU	B	257	19.664	-9.056	32.108	1.00	32.03
ATOM	4847	O	GLU	B	257	16.616	-12.085	28.510	1.00	17.69
ATOM	4848	N	ALA	B	258	16.374	-13.182	29.042	1.00	18.75
ATOM	4849	CA	ALA	B	258	16.262	-11.808	27.256	1.00	17.24
ATOM	4850	CB	ALA	B	258	15.558	-12.786	26.423	1.00	18.43
ATOM	4851	C	ALA	B	258	14.079	-12.680	26.654	1.00	22.18
ATOM	4852	O	ALA	B	258	15.840	-12.507	24.966	1.00	19.20
ATOM	4853	N	GLY	B	259	16.180	-11.370	24.609	1.00	19.32
ATOM	4854	CA	GLY	B	259	15.713	-13.539	24.130	1.00	18.97
ATOM	4855	CB	GLY	B	259	15.917	-13.346	22.700	1.00	18.87
ATOM	4856	O	GLY	B	259	14.894	-12.358	22.161	1.00	19.04
ATOM	4857	N	CYS	B	260	13.693	-12.468	22.453	1.00	18.24
ATOM	4858	CA	CYS	B	260	15.356	-11.389	21.375	1.00	17.25
ATOM	4859	CB	CYS	B	260	14.439	-10.387	20.846	1.00	18.30
ATOM	4860	CG	CYS	B	260	15.216	-9.341	20.048	1.00	17.26
ATOM	4861	SG	CYS	B	260	14.169	-7.950	19.540	1.00	23.04
ATOM	4862	C	CYS	B	260	13.335	-10.980	19.981	1.00	17.67
ATOM	4863	O	CYS	B	260	12.164	-10.678	20.188	1.00	18.38
ATOM	4864	N	ASP	B	261	13.694	-11.811	19.006	1.00	18.04
ATOM	4865	CA	ASP	B	261	12.666	-12.364	18.140	1.00	18.32

Figure 1 (continued 49)

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ATOM	4966	CB	SER	B	274	-4.556	-7.906	23.686	1.00	17.37
ATOM	4967	OG	SER	B	274	-4.390	-7.180	22.474	1.00	17.38
ATOM	4968	C	SER	B	274	-7.033	-7.796	23.318	1.00	17.71
ATOM	4969	O	SER	B	274	-7.542	-7.858	22.189	1.00	17.27
ATOM	4970	N	ASN	B	275	-7.464	-6.965	24.260	1.00	17.56
ATOM	4971	CA	ASN	B	275	-8.550	-6.014	24.026	1.00	18.55
ATOM	4972	CB	ASN	B	275	-8.705	-5.145	25.269	1.00	17.80
ATOM	4973	CG	ASN	B	275	-9.904	-4.223	25.180	1.00	19.42
ATOM	4974	OD1	ASN	B	275	-9.934	-3.339	24.331	1.00	19.77
ATOM	4975	ND2	ASN	B	275	-10.898	-4.431	26.063	1.00	22.03
ATOM	4976	C	ASN	B	275	-8.184	-5.166	22.792	1.00	20.76
ATOM	4977	O	ASN	B	275	-7.090	-4.585	22.723	1.00	17.98
ATOM	4978	N	GLU	B	276	-9.091	-5.093	21.816	1.00	21.76
ATOM	4979	CA	GLU	B	276	-8.779	-4.365	20.591	1.00	23.72
ATOM	4980	CB	GLU	B	276	-9.897	-4.556	19.554	1.00	25.43
ATOM	4981	CG	GLU	B	276	-9.852	-5.932	18.891	1.00	29.37
ATOM	4982	CD	GLU	B	276	-11.021	-6.196	17.960	1.00	32.27
ATOM	4983	OE1	GLU	B	276	-11.600	-5.217	17.442	1.00	33.37
ATOM	4984	OE2	GLU	B	276	-11.348	-7.390	17.745	1.00	32.65
ATOM	4985	C	GLU	B	276	-8.481	-2.888	20.782	1.00	23.01
ATOM	4986	O	GLU	B	276	-7.749	-2.292	19.986	1.00	23.94
ATOM	4987	N	LYS	B	277	-9.034	-2.310	21.837	1.00	23.05
ATOM	4988	CA	LYS	B	277	-8.810	-0.910	22.113	1.00	23.82
ATOM	4989	CB	LYS	B	277	-10.085	-0.230	22.638	1.00	25.13
ATOM	4990	CG	LYS	B	277	-9.852	1.262	22.949	1.00	28.98
ATOM	4991	CD	LYS	B	277	-11.084	2.016	23.463	1.00	31.73
ATOM	4992	CE	LYS	B	277	-10.744	3.512	23.598	1.00	33.68
ATOM	4993	NZ	LYS	B	277	-11.577	4.222	24.623	1.00	35.35
ATOM	4994	C	LYS	B	277	-7.681	-0.655	23.104	1.00	23.58
ATOM	4995	O	LYS	B	277	-6.790	-0.162	22.825	1.00	23.95
ATOM	4996	N	PHE	B	278	-7.702	-1.352	24.244	1.00	21.16
ATOM	4997	CA	PHE	B	278	-6.698	-1.155	25.300	1.00	20.62
ATOM	4998	CB	PHE	B	278	-7.318	-1.432	26.663	1.00	21.99
ATOM	4999	CG	PHE	B	278	-8.431	-0.459	27.021	1.00	26.60
ATOM	5000	CD1	PHE	B	278	-8.142	0.882	27.268	1.00	29.14
ATOM	5001	CD2	PHE	B	278	-9.760	-0.869	27.021	1.00	28.88
ATOM	5002	CE1	PHE	B	278	-9.177	1.816	27.508	1.00	30.11
ATOM	5003	CE2	PHE	B	278	-10.795	0.052	27.258	1.00	30.65
ATOM	5004	CZ	PHE	B	278	-10.496	1.391	27.500	1.00	30.56
ATOM	5005	C	PHE	B	278	-5.403	-1.957	25.131	1.00	19.25
ATOM	5006	O	PHE	B	278	-4.356	-1.582	25.677	1.00	18.94
ATOM	5007	N	ARG	B	279	-5.484	-3.045	24.371	1.00	19.60
ATOM	5008	CA	ARG	B	279	-4.307	-3.865	24.050	1.00	18.45
ATOM	5009	CB	ARG	B	279	-3.404	-3.067	23.088	1.00	19.81
ATOM	5010	CG	ARG	B	279	-4.078	-2.674	21.767	1.00	19.94
ATOM	5011	CD	ARG	B	279	-4.097	-3.843	20.776	1.00	21.13
ATOM	5012	NE	ARG	B	279	-2.777	-3.988	20.175	1.00	23.76
ATOM	5013	CZ	ARG	B	279	-2.423	-4.973	19.365	1.00	22.43
ATOM	5014	NH1	ARG	B	279	-3.297	-5.921	19.058	1.00	25.01
ATOM	5015	NH2	ARG	B	279	-1.202	-4.987	18.838	1.00	23.93
ATOM	5016	C	ARG	B	279	-3.460	-4.360	25.210	1.00	18.23
ATOM	5017	O	ARG	B	279	-2.261	-4.590	25.046	1.00	16.99
ATOM	5018	N	GLY	B	280	-4.062	-4.589	26.365	1.00	16.92
ATOM	5019	CA	GLY	B	280	-3.260	-5.011	27.491	1.00	15.52
ATOM	5020	CB	GLY	B	280	-2.864	-6.477	27.534	1.00	14.43
ATOM	5021	C	GLY	B	280	-3.652	-7.360	27.199	1.00	15.18
ATOM	5022	N	VAL	B	281	-1.623	-6.709	27.942	1.00	15.08
ATOM	5023	CA	VAL	B	281	-1.104	-8.062	28.125	1.00	14.23
ATOM	5024	CB	VAL	B	281	-0.046	-8.473	27.057	1.00	12.60
ATOM	5025	CG1	VAL	B	281	-0.707	-8.654	25.727	1.00	17.31
ATOM	5026	CG2	VAL	B	281	1.061	-7.440	26.981	1.00	15.23
ATOM	5027	C	VAL	B	281	-0.450	-8.059	29.497	1.00	13.94
ATOM	5028	O	VAL	B	281	-0.049	-7.000	30.034	1.00	14.27
ATOM	5029	N	ARG	B	282	-0.387	-9.241	30.091	1.00	12.68
ATOM	5030	CA	ARG	B	282	-0.202	-9.381	31.405	1.00	14.01
ATOM	5031	CB	ARG	B	282	-0.753	-10.142	32.337	1.00	18.49
ATOM	5032	CG	ARG	B	282	-1.999	-9.373	32.712	1.00	25.67
ATOM	5033	CD	ARG	B	282	-2.770	-10.154	33.784	1.00	31.13
ATOM	5034	NE	ARG	B	282	-3.601	-9.274	34.606	1.00	36.93
ATOM	5035	CZ	ARG	B	282	-3.765	-9.449	35.908	1.00	38.95
ATOM	5036	NH1	ARG	B	282	-3.154	-10.470	36.510	1.00	41.34
ATOM	5037	NH2	ARG	B	282	-4.511	-8.605	36.615	1.00	42.07
ATOM	5038	C	ARG	B	282	1.489	-10.168	31.273	1.00	13.94
ATOM	5039	O	ARG	B	282	1.568	-11.118	30.483	1.00	13.78
ATOM	5040	N	LEU	B	283	2.503	-9.736	32.016	1.00	11.77
ATOM	5041	CA	LEU	B	283	3.784	-10.427	32.050	1.00	12.94
ATOM	5042	CB	LEU	B	283	4.931	-9.460	31.806	1.00	13.78
ATOM	5043	CG	LEU	B	283	5.246	-9.059	30.376	1.00	16.55
ATOM	5044	CD1	LEU	B	283	4.078	-8.291	29.772	1.00	18.52
ATOM	5045	CD2	LEU	B	283	6.512	-8.199	30.417	1.00	15.82
ATOM	5046	C	LEU	B	283	3.989	-10.979	33.454	1.00	13.65
ATOM	5047	O	LEU	B	283	3.832	-10.232	34.422	1.00	15.26
ATOM	5048	N	TYR	B	284	4.281	-12.271	33.584	1.00	13.05
ATOM	5049	CA	TYR	B	284	4.580	-12.809	34.913	1.00	13.63
ATOM	5050	CB	TYR	B	284	3.686	-14.004	35.283	1.00	13.56
ATOM	5051	CG	TYR	B	284	3.808	-14.302	36.781	1.00	18.42
ATOM	5052	CD1	TYR	B	284	2.898	-13.778	37.698	1.00	20.54
ATOM	5053	CD2	TYR	B	284	3.069	-13.971	39.101	1.00	22.11
ATOM	5054	CE1	TYR	B	284	4.890	-15.024	37.260	1.00	19.69
ATOM	5055	CE2	TYR	B	284	5.088	-15.221	38.628	1.00	20.37
ATOM	5056	CZ	TYR	B	284	4.175	-14.694	39.544	1.00	22.54
ATOM	5057	OH	TYR	B	284	4.412	-14.897	40.889	1.00	21.81
ATOM	5058	C	TYR	B	284	6.027	-13.271	34.818	1.00	12.58
ATOM	5059	O	TYR	B	284	6.357	-14.144	34.026	1.00	13.78
ATOM	5060	N	VAL	B	285	6.898	-12.675	35.635	1.00	12.36
ATOM	5061	CA	VAL	B	285	8.306	-12.990	35.601	1.00	13.80
ATOM	5062	CB	VAL	B	285	9.106	-11.669	35.724	1.00	16.86
ATOM	5063	CG1	VAL	B	285	10.576	-11.922	35.640	1.00	20.79
ATOM	5064	CG2	VAL	B	285	8.675	-10.718	34.599	1.00	19.51
ATOM	5065	C	VAL	B	285	8.656	-13.928	36.761	1.00	12.81

Figure 1 (continued 51)

ATOM	5066	O	VAL	B	285	8.313	-13.643	37.889	1.00	14.44	B
ATOM	5067	N	SER	B	286	9.318	-15.036	36.464	1.00	13.79	B
ATOM	5068	CA	SER	B	286	9.730	-15.996	37.493	1.00	14.29	B
ATOM	5069	CB	SER	B	286	8.716	-17.148	37.609	1.00	14.83	B
ATOM	5070	OG	SER	B	286	8.623	-17.928	36.439	1.00	17.73	B
ATOM	5071	C	SER	B	286	11.145	-16.492	37.139	1.00	14.68	B
ATOM	5072	O	SER	B	286	11.712	-16.116	36.103	1.00	14.34	B
ATOM	5073	N	GLU	B	287	11.732	-17.338	37.971	1.00	15.06	B
ATOM	5074	CA	GLU	B	287	13.112	-17.732	37.692	1.00	16.29	B
ATOM	5075	CB	GLU	B	287	13.621	-18.691	38.764	1.00	16.48	B
ATOM	5076	CG	GLU	B	287	15.094	-19.065	38.591	1.00	20.87	B
ATOM	5077	CD	GLU	B	287	15.613	-19.806	39.813	1.00	24.94	B
ATOM	5078	OE1	GLU	B	287	15.225	-20.975	40.008	1.00	28.92	B
ATOM	5079	OE2	GLU	B	287	16.400	-19.205	40.580	1.00	32.02	B
ATOM	5080	C	GLU	B	287	13.278	-18.314	36.296	1.00	15.72	B
ATOM	5081	O	GLU	B	287	12.644	-19.303	35.921	1.00	15.04	B
ATOM	5082	N	ASN	B	288	14.134	-17.655	35.518	1.00	14.89	B
ATOM	5083	CA	ASN	B	288	14.386	-18.021	34.127	1.00	15.81	B
ATOM	5084	CB	ASN	B	288	15.363	-19.200	34.049	1.00	17.29	B
ATOM	5085	CG	ASN	B	288	16.736	-18.812	34.607	1.00	19.00	B
ATOM	5086	OD1	ASN	B	288	17.095	-17.642	34.575	1.00	18.60	B
ATOM	5087	ND2	ASN	B	288	17.496	-19.779	35.122	1.00	22.68	B
ATOM	5088	C	ASN	B	288	13.146	-18.280	33.271	1.00	14.61	B
ATOM	5089	O	ASN	B	288	13.196	-19.064	32.325	1.00	15.72	B
ATOM	5090	N	GLN	B	289	12.047	-17.592	33.589	1.00	12.93	B
ATOM	5091	CA	GLN	B	289	10.834	-17.771	32.806	1.00	13.30	B
ATOM	5092	CB	GLN	B	289	9.979	-18.907	33.380	1.00	14.55	B
ATOM	5093	CG	GLN	B	289	8.664	-19.147	32.605	1.00	18.51	B
ATOM	5094	CD	GLN	B	289	7.737	-20.171	33.274	1.00	20.32	B
ATOM	5095	OE1	GLN	B	289	6.714	-19.820	33.912	1.00	24.66	B
ATOM	5096	NE2	GLN	B	289	8.084	-21.430	33.128	1.00	20.90	B
ATOM	5097	C	GLN	B	289	9.950	-16.543	32.706	1.00	13.31	B
ATOM	5098	O	GLN	B	289	9.796	-15.783	33.648	1.00	11.95	B
ATOM	5099	N	LEU	B	290	9.382	-16.347	31.513	1.00	12.64	B
ATOM	5100	CA	LEU	B	290	8.438	-15.253	31.315	1.00	13.02	B
ATOM	5101	CB	LEU	B	290	8.990	-14.220	30.294	1.00	14.05	B
ATOM	5102	CG	LEU	B	290	7.961	-13.160	29.861	1.00	15.71	B
ATOM	5103	CD1	LEU	B	290	7.482	-12.331	31.070	1.00	17.91	B
ATOM	5104	CD2	LEU	B	290	8.586	-12.240	28.816	1.00	17.17	B
ATOM	5105	C	LEU	B	290	7.155	-15.864	30.777	1.00	12.56	B
ATOM	5106	O	LEU	B	290	7.201	-16.657	29.836	1.00	14.23	B
ATOM	5107	N	LYS	B	291	6.022	-15.521	31.391	1.00	12.00	B
ATOM	5108	CA	LYS	B	291	4.723	-15.991	30.909	1.00	12.78	B
ATOM	5109	CB	LYS	B	291	3.958	-16.744	32.014	1.00	14.55	B
ATOM	5110	CG	LYS	B	291	2.521	-17.061	31.604	1.00	17.33	B
ATOM	5111	CD	LYS	B	291	1.794	-17.803	32.734	1.00	23.96	B
ATOM	5112	CE	LYS	B	291	0.313	-17.910	32.428	1.00	28.19	B
ATOM	5113	NZ	LYS	B	291	-0.532	-18.367	33.595	1.00	33.90	B
ATOM	5114	C	LYS	B	291	3.975	-14.725	30.480	1.00	13.62	B
ATOM	5115	O	LYS	B	291	3.869	-13.757	31.243	1.00	15.74	B
ATOM	5116	N	ILE	B	292	3.487	-14.708	29.241	1.00	11.68	B
ATOM	5117	CA	ILE	B	292	2.736	-13.572	28.712	1.00	12.10	B
ATOM	5118	CB	ILE	B	292	3.318	-13.132	27.329	1.00	12.34	B
ATOM	5119	CG2	ILE	B	292	2.448	-12.013	26.690	1.00	14.58	B
ATOM	5120	OG1	ILE	B	292	4.739	-12.646	27.525	1.00	15.22	B
ATOM	5121	CD1	ILE	B	292	5.529	-12.532	26.240	1.00	17.04	B
ATOM	5122	C	ILE	B	292	1.303	-14.048	28.511	1.00	12.60	B
ATOM	5123	O	ILE	B	292	1.075	-15.065	27.844	1.00	13.06	B
ATOM	5124	N	THR	B	293	0.340	-13.316	29.072	1.00	12.37	B
ATOM	5125	CA	THR	B	293	-1.050	-13.703	28.891	1.00	13.44	B
ATOM	5126	CB	THR	B	293	-1.699	-14.182	30.200	1.00	14.23	B
ATOM	5127	OG1	THR	B	293	-1.641	-13.160	31.179	1.00	18.90	B
ATOM	5128	CG2	THR	B	293	-0.947	-15.366	30.766	1.00	15.88	B
ATOM	5129	C	THR	B	293	-1.832	-12.535	28.372	1.00	14.34	B
ATOM	5130	O	THR	B	293	-1.471	-11.362	28.600	1.00	13.84	B
ATOM	5131	N	ALA	B	294	-2.883	-12.837	27.634	1.00	12.99	B
ATOM	5132	CA	ALA	B	294	-3.746	-11.800	27.101	1.00	14.01	B
ATOM	5133	CB	ALA	B	294	-3.325	-11.469	25.644	1.00	15.00	B
ATOM	5134	C	ALA	B	294	-5.164	-12.333	27.116	1.00	15.21	B
ATOM	5135	O	ALA	B	294	-5.383	-13.509	26.864	1.00	15.46	B
ATOM	5136	N	ASN	B	295	-6.132	-11.486	27.461	1.00	15.97	B
ATOM	5137	CA	ASN	B	295	-7.515	-11.907	27.367	1.00	17.95	B
ATOM	5138	CB	ASN	B	295	-8.052	-12.461	28.700	1.00	23.39	B
ATOM	5139	CG	ASN	B	295	-8.003	-11.480	29.817	1.00	25.82	B
ATOM	5140	OD1	ASN	B	295	-8.523	-10.373	29.718	1.00	31.67	B
ATOM	5141	ND2	ASN	B	295	-7.393	-11.888	30.929	1.00	32.50	B
ATOM	5142	C	ASN	B	295	-8.325	-10.718	26.865	1.00	16.88	B
ATOM	5143	O	ASN	B	295	-7.873	-9.568	26.935	1.00	17.31	B
ATOM	5144	N	ASN	B	296	-9.499	-10.996	26.302	1.00	16.35	B
ATOM	5145	CA	ASN	B	296	-10.311	-9.920	25.755	1.00	17.61	B
ATOM	5146	CB	ASN	B	296	-10.294	-9.966	24.205	1.00	16.78	B
ATOM	5147	CG	ASN	B	296	-10.835	-11.274	23.639	1.00	17.58	B
ATOM	5148	OD1	ASN	B	296	-11.629	-11.955	24.285	1.00	19.52	B
ATOM	5149	ND2	ASN	B	296	-10.438	-11.601	22.407	1.00	18.80	B
ATOM	5150	C	ASN	B	296	-11.734	-10.022	26.306	1.00	18.87	B
ATOM	5151	O	ASN	B	296	-12.049	-10.878	27.141	1.00	18.85	B
ATOM	5152	N	PRO	B	297	-12.603	-9.111	25.877	1.00	22.70	B
ATOM	5153	CD	PRO	B	297	-12.351	-7.873	25.120	1.00	23.09	B
ATOM	5154	CA	PRO	B	297	-13.975	-9.157	26.373	1.00	25.09	B
ATOM	5155	CB	PRO	B	297	-14.586	-7.858	25.842	1.00	25.02	B
ATOM	5156	CG	PRO	B	297	-13.432	-6.952	25.666	1.00	23.49	B
ATOM	5157	C	PRO	B	297	-14.773	-10.376	25.925	1.00	26.91	B
ATOM	5158	O	PRO	B	297	-15.828	-10.638	26.490	1.00	29.58	B
ATOM	5159	N	GLU	B	298	-14.317	-11.085	24.893	1.00	28.28	B
ATOM	5160	CA	GLU	B	298	-15.033	-12.275	24.425	1.00	29.32	B
ATOM	5161	CB	GLU	B	298	-14.805	-12.487	22.919	1.00	33.72	B
ATOM	5162	CG	GLU	B	298	-15.968	-12.033	22.025	1.00	38.43	B
ATOM	5163	CD	GLU	B	298	-16.282	-10.547	22.144	1.00	42.52	B
ATOM	5164	OE1	GLU	B	298	-15.362	-9.730	21.889	1.00	43.73	B
ATOM	5165	OE2	GLU	B	298	-17.449	-10.200	22.490	1.00	43.97	B

Figure 1 (continued 52)

[illegible]

Figure 1 (continued 53)

ATOM	5266	C	TYR	B	310	16.202	-14.605	36.635	1.00	20.33
ATOM	5267	O	TYR	B	310	15.861	-15.775	36.802	1.00	18.99
ATOM	5268	N	SER	B	311	16.711	-13.831	37.604	1.00	21.68
ATOM	5269	CA	SER	B	311	16.890	-14.340	38.973	1.00	25.75
ATOM	5270	CB	SER	B	311	18.376	-14.490	39.291	1.00	27.17
ATOM	5271	OG	SER	B	311	18.819	-15.761	38.877	1.00	32.61
ATOM	5272	C	SER	B	311	16.229	-13.539	40.094	1.00	27.05
ATOM	5273	O	GLY	B	312	15.500	-13.876	41.264	1.00	31.83
ATOM	5274	N	GLY	B	312	14.864	-12.481	39.778	1.00	28.46
ATOM	5275	CA	GLY	B	312	13.588	-12.299	41.478	1.00	27.94
ATOM	5276	CB	ALA	B	313	13.187	-13.451	41.239	1.00	26.97
ATOM	5277	O	ALA	B	313	12.957	-11.478	42.310	1.00	26.88
ATOM	5278	N	ALA	B	313	11.711	-11.848	42.966	1.00	24.05
ATOM	5279	CA	ALA	B	313	11.312	-10.763	43.966	1.00	24.56
ATOM	5280	CB	GLU	B	314	10.665	-11.932	41.853	1.00	22.56
ATOM	5281	C	GLU	B	314	10.806	-11.298	40.799	1.00	20.08
ATOM	5282	O	GLU	B	314	9.618	-12.725	42.066	1.00	19.40
ATOM	5283	N	GLU	B	314	8.586	-12.840	41.042	1.00	18.07
ATOM	5284	CA	GLU	B	314	7.647	-14.039	41.323	1.00	16.92
ATOM	5285	CB	GLU	B	314	8.410	-15.354	41.405	1.00	16.41
ATOM	5286	CG	GLU	B	314	7.525	-16.589	41.365	1.00	14.40
ATOM	5287	CD	GLU	B	314	6.317	-16.485	41.643	1.00	15.57
ATOM	5288	OE1	GLU	B	314	8.058	-17.668	41.064	1.00	17.05
ATOM	5289	OE2	GLU	B	314	7.772	-11.565	41.032	1.00	17.69
ATOM	5290	C	MET	B	315	7.685	-10.870	42.033	1.00	18.99
ATOM	5291	O	MET	B	315	7.209	-11.226	39.878	1.00	18.30
ATOM	5292	N	MET	B	315	6.352	-10.044	39.793	1.00	16.99
ATOM	5293	CA	MET	B	315	7.156	-8.741	39.754	1.00	19.43
ATOM	5294	CB	MET	B	315	8.052	-8.587	38.571	1.00	18.90
ATOM	5295	CG	MET	B	315	8.654	-6.862	38.490	1.00	23.78
ATOM	5296	SD	MET	B	315	7.247	-6.033	37.765	1.00	21.20
ATOM	5297	CE	MET	B	315	5.509	-10.144	38.542	1.00	18.24
ATOM	5298	C	GLU	B	316	5.833	-10.890	37.618	1.00	16.64
ATOM	5299	O	GLU	B	316	4.404	-9.423	38.554	1.00	17.91
ATOM	5300	N	GLU	B	316	3.499	-9.387	37.442	1.00	19.14
ATOM	5301	CA	GLU	B	316	2.153	-9.964	37.876	1.00	22.45
ATOM	5302	CB	GLU	B	316	1.183	-10.293	36.755	1.00	30.42
ATOM	5303	CG	GLU	B	316	-0.058	-11.022	37.282	1.00	33.19
ATOM	5304	CD	GLU	B	316	-0.126	-12.269	37.189	1.00	36.29
ATOM	5305	OE1	GLU	B	316	-0.957	-10.337	37.807	1.00	35.89
ATOM	5306	OE2	GLU	B	316	3.374	-7.916	37.058	1.00	18.61
ATOM	5307	C	ILE	B	317	3.442	-7.029	37.917	1.00	19.48
ATOM	5308	O	ILE	B	317	3.202	-7.651	35.770	1.00	17.17
ATOM	5309	N	ILE	B	317	3.090	-6.281	35.317	1.00	14.40
ATOM	5310	CA	ILE	B	317	4.500	-5.648	35.163	1.00	15.39
ATOM	5311	CB	ILE	B	317	5.382	-6.449	34.724	1.00	16.07
ATOM	5312	CG1	ILE	B	317	4.373	-4.195	34.830	1.00	16.39
ATOM	5313	CG2	ILE	B	317	5.731	-3.450	34.003	1.00	15.91
ATOM	5314	CD1	ILE	B	317	2.319	-6.249	33.166	1.00	15.36
ATOM	5315	C	GLY	B	318	2.484	-7.144	33.826	1.00	15.37
ATOM	5316	O	GLY	B	318	1.489	-5.225	32.611	1.00	13.91
ATOM	5317	N	GLY	B	318	0.701	-5.121	31.670	1.00	15.48
ATOM	5318	CA	PHE	B	319	1.261	-4.061	32.135	1.00	14.18
ATOM	5319	CB	PHE	B	319	1.888	-3.115	30.363	1.00	15.89
ATOM	5320	O	PHE	B	319	1.072	-4.255	28.777	1.00	16.03
ATOM	5321	N	PHE	B	319	1.513	-3.311	29.877	1.00	17.13
ATOM	5322	CA	PHE	B	319	2.897	-3.692	30.368	1.00	21.89
ATOM	5323	CB	PHE	B	319	4.022	-3.383	30.740	1.00	22.47
ATOM	5324	CG	PHE	B	319	4.434	-2.073	31.236	1.00	21.80
ATOM	5325	CD1	PHE	B	319	4.673	-4.401	31.423	1.00	23.74
ATOM	5326	CD2	PHE	B	319	5.481	-1.786	28.129	1.00	16.79
ATOM	5327	OE1	PHE	B	319	5.716	-4.122	27.846	1.00	16.27
ATOM	5328	OE2	PHE	B	319	6.121	-2.820	26.158	1.00	16.46
ATOM	5329	CZ	PHE	B	319	0.602	-3.282	25.796	1.00	18.69
ATOM	5330	C	ASN	B	320	-0.122	-4.242	24.407	1.00	18.32
ATOM	5331	O	ASN	B	320	0.635	-2.143	23.481	1.00	18.44
ATOM	5332	N	ASN	B	320	-0.051	-1.983	24.242	1.00	17.08
ATOM	5333	CA	ASN	B	320	-0.055	-0.504	25.102	1.00	16.27
ATOM	5334	CB	ASN	B	320	-0.561	-0.259	23.845	1.00	15.94
ATOM	5335	CG	ASN	B	320	-0.226	-0.997	23.464	1.00	16.35
ATOM	5336	OD1	ASN	B	320	-1.362	0.791	22.450	1.00	17.69
ATOM	5337	ND2	ASN	B	320	0.927	-2.745	22.956	1.00	14.64
ATOM	5338	C	VAL	B	321	2.093	-2.350	22.610	1.00	17.10
ATOM	5339	O	VAL	B	321	0.478	-3.843	22.119	1.00	15.35
ATOM	5340	N	VAL	B	321	1.379	-4.662	22.109	1.00	16.12
ATOM	5341	CA	VAL	B	321	0.703	-6.027	20.925	1.00	17.12
ATOM	5342	CB	VAL	B	321	-0.409	-5.817	19.863	1.00	18.39
ATOM	5343	CG1	VAL	B	321	1.743	-7.004	21.276	1.00	15.98
ATOM	5344	CG2	VAL	B	321	1.891	-3.939	22.482	1.00	15.16
ATOM	5345	C	TYR	B	322	2.977	-4.245	22.908	1.00	14.24
ATOM	5346	O	TYR	B	322	1.146	-2.961	24.259	1.00	15.80
ATOM	5347	N	TYR	B	322	1.657	-2.257	24.294	1.00	15.47
ATOM	5348	CA	TYR	B	322	0.587	-1.352	23.127	1.00	16.25
ATOM	5349	CB	TYR	B	322	-0.513	-2.129	23.170	1.00	20.04
ATOM	5350	CG	TYR	B	322	2.899	-1.436	25.509	1.00	18.22
ATOM	5351	O	TYR	B	322	3.837	-1.353	24.399	1.00	19.75
ATOM	5352	N	TYR	B	322	2.932	-0.853	24.453	1.00	21.19
ATOM	5353	CA	TYR	B	323	4.110	-0.088	23.041	1.00	23.64
ATOM	5354	CB	TYR	B	323	3.878	0.590	22.726	1.00	15.80
ATOM	5355	CG	TYR	B	323	2.813	1.668	23.563	1.00	15.87
ATOM	5356	CD1	TYR	B	323	2.397	2.314			
ATOM	5357	CD2	TYR	B	323	1.458	3.374			
ATOM	5358	CE1	TYR	B	323	2.284	2.093			
ATOM	5359	CE2	TYR	B	323	1.354	3.166			
ATOM	5360	CZ	TYR	B	323	0.957	3.790			
ATOM	5361	OH	TYR	B	323	0.112	4.886			
ATOM	5362	C	TYR	B	323	5.327	-1.018			
ATOM	5363	O	TYR	B	323	6.468	-0.646			
ATOM	5364	N	VAL	B	324	5.101	-2.226			
ATOM	5365									

Figure 1 (continued 54)

ATOM	5366	CA	VAL	B	324	6.193	-3.182	23.687	1.00	14.69
ATOM	5367	CB	VAL	B	324	5.776	-4.387	24.550	1.00	14.90
ATOM	5368	CG1	VAL	B	324	6.913	-5.422	24.610	1.00	16.80
ATOM	5369	CG2	VAL	B	324	5.440	-3.896	25.952	1.00	16.82
ATOM	5370	C	VAL	B	324	6.674	-3.670	22.301	1.00	13.75
ATOM	5371	N	VAL	B	324	7.885	-3.761	22.039	1.00	14.44
ATOM	5372	O	LEU	B	325	5.737	-3.984	21.410	1.00	14.44
ATOM	5373	CA	LEU	B	325	6.105	-4.424	20.085	1.00	13.52
ATOM	5374	CB	LEU	B	325	4.852	-4.870	19.317	1.00	14.38
ATOM	5375	CG	LEU	B	325	4.339	-6.244	19.774	1.00	14.30
ATOM	5376	CD1	LEU	B	325	2.953	-6.506	19.170	1.00	15.19
ATOM	5377	CD2	LEU	B	325	5.338	-7.346	19.363	1.00	14.63
ATOM	5378	C	LEU	B	325	6.848	-3.319	19.334	1.00	14.06
ATOM	5379	O	LEU	B	325	7.801	-3.603	18.606	1.00	15.63
ATOM	5380	N	ASP	B	326	6.420	-2.074	19.503	1.00	14.14
ATOM	5381	CA	ASP	B	326	7.113	-0.960	18.843	1.00	14.45
ATOM	5382	CB	ASP	B	326	6.505	0.385	19.217	1.00	15.89
ATOM	5383	CG	ASP	B	326	5.168	0.634	18.556	1.00	16.26
ATOM	5384	OD1	ASP	B	326	4.803	-0.036	17.556	1.00	17.26
ATOM	5385	OD2	ASP	B	326	4.471	1.551	19.018	1.00	18.69
ATOM	5386	C	ASP	B	326	8.588	-0.952	19.255	1.00	14.86
ATOM	5387	O	ASP	B	326	9.454	-0.768	18.416	1.00	15.93
ATOM	5388	N	VAL	B	327	8.871	-1.163	20.542	1.00	15.32
ATOM	5389	CA	VAL	B	327	10.246	-1.175	20.989	1.00	15.55
ATOM	5390	CB	VAL	B	327	10.301	-1.226	22.534	1.00	16.32
ATOM	5391	CG1	VAL	B	327	11.715	-1.474	22.996	1.00	15.81
ATOM	5392	CG2	VAL	B	327	9.783	0.086	23.085	1.00	15.65
ATOM	5393	C	VAL	B	327	11.039	-2.352	20.422	1.00	16.20
ATOM	5394	O	VAL	B	327	12.179	-2.184	19.974	1.00	15.94
ATOM	5395	N	LEU	B	328	10.437	-3.547	20.435	1.00	14.84
ATOM	5396	CA	LEU	B	328	11.150	-4.726	19.961	1.00	15.54
ATOM	5397	CB	LEU	B	328	10.347	-5.985	20.295	1.00	14.62
ATOM	5398	CG	LEU	B	328	10.130	-6.193	21.808	1.00	15.10
ATOM	5399	CD1	LEU	B	328	9.295	-7.460	22.024	1.00	14.68
ATOM	5400	CD2	LEU	B	328	11.503	-6.337	22.497	1.00	16.58
ATOM	5401	C	LEU	B	328	11.416	-4.600	18.480	1.00	16.34
ATOM	5402	O	LEU	B	328	12.455	-5.042	17.998	1.00	17.56
ATOM	5403	N	ASN	B	329	10.491	-3.970	17.758	1.00	17.06
ATOM	5404	CA	ASN	B	329	10.680	-3.755	16.332	1.00	20.23
ATOM	5405	CB	ASN	B	329	9.371	-3.285	15.675	1.00	20.68
ATOM	5406	CG	ASN	B	329	8.414	-4.440	15.381	1.00	25.15
ATOM	5407	OD1	ASN	B	329	7.193	-4.308	15.536	1.00	29.33
ATOM	5408	ND2	ASN	B	329	8.961	-5.571	14.932	1.00	25.44
ATOM	5409	C	ASN	B	329	11.790	-2.743	16.076	1.00	20.26
ATOM	5410	O	ASN	B	329	12.504	-2.875	15.074	1.00	21.57
ATOM	5411	N	ALA	B	330	11.958	-1.754	16.963	1.00	19.54
ATOM	5412	CA	ALA	B	330	13.007	-0.741	16.795	1.00	20.36
ATOM	5413	CB	ALA	B	330	12.703	0.488	17.630	1.00	19.00
ATOM	5414	C	ALA	B	330	14.392	-1.275	17.151	1.00	22.18
ATOM	5415	O	ALA	B	330	15.410	-0.786	16.652	1.00	22.02
ATOM	5416	N	LEU	B	331	14.425	-2.269	18.031	1.00	22.79
ATOM	5417	CA	LEU	B	331	15.675	-2.900	18.445	1.00	26.40
ATOM	5418	CB	LEU	B	331	15.542	-3.459	19.876	1.00	24.34
ATOM	5419	CG	LEU	B	331	15.521	-2.496	21.077	1.00	23.11
ATOM	5420	CD1	LEU	B	331	15.059	-3.251	22.320	1.00	23.07
ATOM	5421	CD2	LEU	B	331	16.904	-1.904	21.324	1.00	22.88
ATOM	5422	C	LEU	B	331	15.953	-4.042	17.466	1.00	29.87
ATOM	5423	O	LEU	B	331	15.346	-5.118	17.543	1.00	32.92
ATOM	5424	N	LYS	B	332	16.871	-3.831	16.540	1.00	32.35
ATOM	5425	CA	LYS	B	332	17.157	-4.892	15.576	1.00	34.77
ATOM	5426	CB	LYS	B	332	17.447	-4.281	14.205	1.00	37.40
ATOM	5427	CG	LYS	B	332	18.504	-3.195	14.249	1.00	41.60
ATOM	5428	CD	LYS	B	332	18.968	-2.812	12.865	1.00	44.04
ATOM	5429	CE	LYS	B	332	20.404	-2.327	12.925	1.00	46.03
ATOM	5430	NZ	LYS	B	332	21.304	-3.408	13.449	1.00	46.84
ATOM	5431	C	LYS	B	332	18.364	-5.647	16.110	1.00	34.26
ATOM	5432	O	LYS	B	332	19.478	-5.520	15.583	1.00	36.38
ATOM	5433	N	CYS	B	333	18.139	-6.428	17.167	1.00	31.45
ATOM	5434	CA	CYS	B	333	19.227	-7.147	17.809	1.00	28.74
ATOM	5435	CB	CYS	B	333	19.682	-6.364	19.040	1.00	26.65
ATOM	5436	SG	CYS	B	333	18.382	-6.128	20.301	1.00	24.29
ATOM	5437	C	CYS	B	333	18.900	-8.582	18.201	1.00	27.77
ATOM	5438	O	CYS	B	333	17.771	-9.039	18.057	1.00	27.74
ATOM	5439	N	GLU	B	334	19.891	-9.292	18.722	1.00	24.94
ATOM	5440	CA	GLU	B	334	19.651	-10.671	19.072	1.00	25.13
ATOM	5441	CB	GLU	B	334	20.940	-11.490	19.059	1.00	28.75
ATOM	5442	CG	GLU	B	334	20.639	-12.973	18.832	1.00	33.58
ATOM	5443	CD	GLU	B	334	21.798	-13.903	19.171	1.00	37.85
ATOM	5444	OE1	GLU	B	334	22.835	-13.880	18.469	1.00	38.76
ATOM	5445	OE2	GLU	B	334	21.656	-14.670	20.151	1.00	39.90
ATOM	5446	C	GLU	B	334	18.977	-10.831	20.420	1.00	22.72
ATOM	5447	O	GLU	B	334	18.060	-11.628	20.559	1.00	22.05
ATOM	5448	N	ASN	B	335	19.449	-10.089	21.410	1.00	21.54
ATOM	5449	CA	ASN	B	335	18.873	-10.202	22.751	1.00	21.37
ATOM	5450	CB	ASN	B	335	19.841	-10.945	23.673	1.00	22.21
ATOM	5451	CG	ASN	B	335	20.230	-12.327	23.127	1.00	23.10
ATOM	5452	OD1	ASN	B	335	21.320	-12.515	22.569	1.00	27.23
ATOM	5453	ND2	ASN	B	335	19.349	-13.283	23.283	1.00	20.66
ATOM	5454	C	ASN	B	335	18.540	-8.849	23.347	1.00	21.05
ATOM	5455	O	ASN	B	335	19.193	-7.848	23.057	1.00	19.95
ATOM	5456	N	VAL	B	336	17.499	-8.824	24.174	1.00	18.30
ATOM	5457	CA	VAL	B	336	17.074	-7.600	24.817	1.00	18.62
ATOM	5458	CB	VAL	B	336	15.629	-7.224	24.418	1.00	19.11
ATOM	5459	CG1	VAL	B	336	15.564	-6.941	22.908	1.00	19.33
ATOM	5460	CG2	VAL	B	336	14.681	-8.367	24.762	1.00	23.69
ATOM	5461	C	VAL	B	336	17.118	-7.770	26.331	1.00	19.78
ATOM	5462	O	VAL	B	336	17.054	-8.896	26.846	1.00	20.30
ATOM	5463	N	ARG	B	337	17.243	-6.644	27.022	1.00	18.96
ATOM	5464	CA	ARG	B	337	17.259	-6.617	28.482	1.00	19.16
ATOM	5465	CB	ARG	B	337	18.589	-6.071	29.016	1.00	20.68

Figure 1 (continued 55)

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Figure 1 (continued 56)

ATOM	5566	CD	GLU	B	350	19.768	-1.317	28.861	1.00	28.87	B
ATOM	5567	OE1	GLU	B	350	19.985	-0.085	28.838	1.00	30.71	B
ATOM	5568	OE2	GLU	B	350	20.435	-2.111	29.569	1.00	32.23	B
ATOM	5569	C	GLU	B	350	18.018	-3.247	25.033	1.00	20.43	B
ATOM	5570	O	GLU	B	350	17.663	-4.385	25.373	1.00	19.39	B
ATOM	5571	N	ASP	B	351	18.864	-3.023	24.030	1.00	18.78	B
ATOM	5572	CA	ASP	B	351	19.556	-4.127	23.383	1.00	20.40	B
ATOM	5573	CB	ASP	B	351	20.393	-3.559	22.216	1.00	20.92	B
ATOM	5574	CG	ASP	B	351	21.276	-4.593	21.540	1.00	24.22	B
ATOM	5575	OD1	ASP	B	351	21.520	-5.668	22.122	1.00	23.24	B
ATOM	5576	OD2	ASP	B	351	21.747	-4.326	20.399	1.00	24.36	B
ATOM	5577	C	ASP	B	351	20.480	-4.641	24.519	1.00	20.22	B
ATOM	5578	O	ASP	B	351	21.154	-3.837	25.166	1.00	19.94	B
ATOM	5579	N	ALA	B	352	20.513	-5.955	24.767	1.00	20.14	B
ATOM	5580	CA	ALA	B	352	21.371	-6.512	25.828	1.00	22.88	B
ATOM	5581	CB	ALA	B	352	21.102	-8.023	25.989	1.00	23.61	B
ATOM	5582	C	ALA	B	352	22.856	-6.282	25.541	1.00	25.05	B
ATOM	5583	O	ALA	B	352	23.687	-6.298	26.459	1.00	25.32	B
ATOM	5584	N	ALA	B	353	23.187	-6.059	24.272	1.00	25.32	B
ATOM	5585	CA	ALA	B	353	24.583	-5.871	23.874	1.00	27.92	B
ATOM	5586	CB	ALA	B	353	24.888	-6.727	22.622	1.00	28.12	B
ATOM	5587	C	ALA	B	353	25.008	-4.429	23.628	1.00	29.48	B
ATOM	5588	O	ALA	B	353	26.134	-4.185	23.189	1.00	30.65	B
ATOM	5589	N	SER	B	354	24.130	-3.471	23.895	1.00	28.82	B
ATOM	5590	CA	SER	B	354	24.491	-2.068	23.695	1.00	30.09	B
ATOM	5591	CB	SER	B	354	24.439	-1.695	22.213	1.00	30.87	B
ATOM	5592	CG	SER	B	354	24.378	-0.282	22.073	1.00	30.83	B
ATOM	5593	C	SER	B	354	23.612	-1.097	24.458	1.00	29.65	B
ATOM	5594	O	SER	B	354	22.382	-1.233	24.488	1.00	29.50	B
ATOM	5595	N	GLN	B	355	24.236	-0.096	25.064	1.00	29.47	B
ATOM	5596	CA	GLN	B	355	23.475	0.900	25.794	1.00	29.78	B
ATOM	5597	CB	GLN	B	355	24.227	1.337	27.057	1.00	33.08	B
ATOM	5598	CG	GLN	B	355	24.449	0.245	28.091	1.00	37.90	B
ATOM	5599	CD	GLN	B	355	25.421	0.691	29.180	1.00	41.35	B
ATOM	5600	OE1	GLN	B	355	26.640	0.756	28.959	1.00	42.13	B
ATOM	5601	NE2	GLN	B	355	24.883	1.026	30.355	1.00	42.11	B
ATOM	5602	C	GLN	B	355	23.230	2.117	24.896	1.00	29.04	B
ATOM	5603	O	GLN	B	355	22.833	3.167	25.389	1.00	29.11	B
ATOM	5604	N	SER	B	356	23.439	1.963	23.586	1.00	28.20	B
ATOM	5605	CA	SER	B	356	23.247	3.072	22.630	1.00	28.53	B
ATOM	5606	CB	SER	B	356	23.499	2.600	21.187	1.00	29.22	B
ATOM	5607	CG	SER	B	356	24.878	2.462	20.908	1.00	33.92	B
ATOM	5608	C	SER	B	356	21.839	3.659	22.699	1.00	26.91	B
ATOM	5609	O	SER	B	356	21.636	4.883	22.644	1.00	26.04	B
ATOM	5610	N	ALA	B	357	20.849	2.782	22.801	1.00	24.78	B
ATOM	5611	CA	ALA	B	357	19.476	3.240	22.852	1.00	23.09	B
ATOM	5612	CB	ALA	B	357	18.707	2.773	21.599	1.00	23.03	B
ATOM	5613	C	ALA	B	357	18.795	2.702	24.099	1.00	23.24	B
ATOM	5614	O	ALA	B	357	19.167	1.646	24.625	1.00	25.22	B
ATOM	5615	N	ALA	B	358	17.825	3.457	24.587	1.00	21.13	B
ATOM	5616	CA	ALA	B	358	17.055	3.030	25.747	1.00	21.52	B
ATOM	5617	CB	ALA	B	358	17.643	3.649	27.031	1.00	22.50	B
ATOM	5618	C	ALA	B	358	15.585	3.402	25.566	1.00	19.54	B
ATOM	5619	O	ALA	B	358	15.257	4.451	25.037	1.00	18.37	B
ATOM	5620	N	TYR	B	359	14.683	2.527	26.017	1.00	18.21	B
ATOM	5621	CA	TYR	B	359	13.259	2.747	25.886	1.00	18.06	B
ATOM	5622	CB	TYR	B	359	12.642	1.724	24.919	1.00	17.72	B
ATOM	5623	CG	TYR	B	359	13.303	1.776	23.558	1.00	15.03	B
ATOM	5624	CD1	TYR	B	359	14.473	1.076	23.300	1.00	16.16	B
ATOM	5625	CE1	TYR	B	359	15.151	1.242	22.104	1.00	14.13	B
ATOM	5626	CD2	TYR	B	359	12.812	2.648	22.573	1.00	15.69	B
ATOM	5627	CE2	TYR	B	359	13.485	2.819	21.379	1.00	13.85	B
ATOM	5628	CZ	TYR	B	359	14.633	2.127	21.145	1.00	15.70	B
ATOM	5629	OH	TYR	B	359	15.265	2.315	19.935	1.00	16.11	B
ATOM	5630	O	TYR	B	359	12.597	2.609	27.235	1.00	19.04	B
ATOM	5631	N	VAL	B	360	12.908	1.686	27.992	1.00	19.57	B
ATOM	5632	CA	VAL	B	360	11.730	3.546	27.545	1.00	17.94	B
ATOM	5633	CB	VAL	B	360	11.023	3.501	28.812	1.00	19.18	B
ATOM	5634	C	VAL	B	360	11.276	4.794	29.641	1.00	18.75	B
ATOM	5635	CG1	VAL	B	360	10.448	4.742	30.934	1.00	20.25	B
ATOM	5636	CG2	VAL	B	360	12.753	4.923	29.937	1.00	19.41	B
ATOM	5637	C	VAL	B	360	9.562	3.381	28.501	1.00	19.10	B
ATOM	5638	O	VAL	B	360	9.008	4.188	27.753	1.00	19.90	B
ATOM	5639	N	VAL	B	361	8.905	2.372	29.069	1.00	19.72	B
ATOM	5640	CA	VAL	B	361	7.488	2.188	28.831	1.00	18.92	B
ATOM	5641	CB	VAL	B	361	7.216	0.872	28.069	1.00	18.99	B
ATOM	5642	CG1	VAL	B	361	5.743	0.769	27.716	1.00	18.31	B
ATOM	5643	CG2	VAL	B	361	8.065	0.839	26.786	1.00	17.76	B
ATOM	5644	C	VAL	B	361	6.793	2.100	30.167	1.00	19.47	B
ATOM	5645	O	VAL	B	361	7.232	1.362	31.038	1.00	16.90	B
ATOM	5646	N	MET	B	362	5.737	2.885	30.318	1.00	20.10	B
ATOM	5647	CA	MET	B	362	4.962	2.882	31.540	1.00	21.78	B
ATOM	5648	CB	MET	B	362	4.226	4.206	31.682	1.00	24.19	B
ATOM	5649	CG	MET	B	362	3.918	4.589	33.122	1.00	27.23	B
ATOM	5650	SD	MET	B	362	5.405	4.806	34.163	1.00	29.11	B
ATOM	5651	CE	MET	B	362	4.575	4.880	35.731	1.00	30.05	B
ATOM	5652	C	MET	B	362	3.949	1.731	31.471	1.00	20.28	B
ATOM	5653	O	MET	B	362	3.385	1.438	30.410	1.00	19.68	B
ATOM	5654	N	PRO	B	363	3.698	1.069	32.599	1.00	20.71	B
ATOM	5655	CA	PRO	B	363	4.521	1.025	33.818	1.00	21.21	B
ATOM	5656	CB	PRO	B	363	2.729	-0.038	32.579	1.00	20.67	B
ATOM	5657	CG	PRO	B	363	3.155	-0.883	33.776	1.00	22.57	B
ATOM	5658	C	PRO	B	363	3.665	0.160	34.754	1.00	22.37	B
ATOM	5659	O	PRO	B	363	1.272	0.395	32.672	1.00	22.28	B
ATOM	5660	N	PRO	B	364	0.959	1.574	32.811	1.00	18.47	B
ATOM	5661	CA	MET	B	364	0.368	-0.568	32.537	1.00	23.87	B
ATOM	5662	CB	MET	B	364	-1.037	-0.272	32.674	1.00	26.94	B
ATOM	5663	CG	MET	B	364	-1.780	-0.391	31.332	1.00	29.59	B
ATOM	5664	SD	MET	B	364	-1.636	-1.670	30.568	1.00	31.24	B
ATOM	5665					-2.386	-1.510	28.872	1.00	31.43	B

Figure 1 (continued 57)

[illegible]

Figure 1 (continued 58)

ATOM	5766	OH2	TIP	S	22	-27.660	-14.486	-13.561	1.00	17.12
ATOM	5767	OH2	TIP	S	23	-13.962	-0.925	-21.605	1.00	14.22
ATOM	5768	OH2	TIP	S	24	1.435	28.503	-10.938	1.00	18.48
ATOM	5769	OH2	TIP	S	25	9.366	3.813	23.519	1.00	16.22
ATOM	5770	OH2	TIP	S	26	6.434	-22.228	22.332	1.00	19.93
ATOM	5771	OH2	TIP	S	27	7.890	-18.056	18.119	1.00	19.57
ATOM	5772	OH2	TIP	S	28	-15.000	8.720	-22.814	1.00	14.68
ATOM	5773	OH2	TIP	S	29	10.776	24.804	-24.045	1.00	16.80
ATOM	5774	OH2	TIP	S	30	1.778	20.791	-6.653	1.00	17.56
ATOM	5775	OH2	TIP	S	31	0.621	20.501	-9.333	1.00	18.49
ATOM	5776	OH2	TIP	S	32	4.572	1.385	-28.353	1.00	18.53
ATOM	5777	OH2	TIP	S	33	8.530	13.438	21.012	1.00	18.38
ATOM	5778	OH2	TIP	S	34	-5.364	-34.951	13.172	1.00	16.54
ATOM	5779	OH2	TIP	S	35	-0.215	-6.534	-30.846	1.00	17.23
ATOM	5780	OH2	TIP	S	36	3.783	18.454	-29.707	1.00	19.51
ATOM	5781	OH2	TIP	S	37	3.591	-1.199	-27.445	1.00	19.45
ATOM	5782	OH2	TIP	S	38	9.369	34.981	-11.888	1.00	20.02
ATOM	5783	OH2	TIP	S	39	10.133	-20.154	36.900	1.00	17.90
ATOM	5784	OH2	TIP	S	40	3.793	8.403	-19.080	1.00	16.65
ATOM	5785	OH2	TIP	S	41	10.939	4.680	14.536	1.00	18.20
ATOM	5786	OH2	TIP	S	42	8.076	12.297	-25.798	1.00	16.16
ATOM	5787	OH2	TIP	S	43	-14.372	-32.728	6.563	1.00	18.38
ATOM	5788	OH2	TIP	S	44	-23.715	-9.227	-23.646	1.00	21.11
ATOM	5789	OH2	TIP	S	45	20.825	28.255	-9.159	1.00	16.67
ATOM	5790	OH2	TIP	S	46	-1.109	13.957	-40.824	1.00	17.50
ATOM	5791	OH2	TIP	S	47	5.330	-27.571	17.233	1.00	20.27
ATOM	5792	OH2	TIP	S	48	-6.283	-7.101	26.866	1.00	19.83
ATOM	5793	OH2	TIP	S	49	-4.904	-9.220	29.033	1.00	18.63
ATOM	5794	OH2	TIP	S	50	6.596	25.027	-2.197	1.00	18.25
ATOM	5795	OH2	TIP	S	51	3.946	-28.513	19.328	1.00	22.98
ATOM	5796	OH2	TIP	S	52	18.496	30.057	13.872	1.00	21.35
ATOM	5797	OH2	TIP	S	53	14.476	13.406	-26.031	1.00	20.88
ATOM	5798	OH2	TIP	S	54	-5.854	17.119	-30.322	1.00	18.67
ATOM	5799	OH2	TIP	S	55	-11.444	-12.723	13.885	1.00	21.78
ATOM	5800	OH2	TIP	S	56	-18.531	-23.945	-2.069	1.00	20.92
ATOM	5801	OH2	TIP	S	57	8.793	-1.749	36.685	1.00	23.51
ATOM	5802	OH2	TIP	S	58	-10.518	17.199	-18.634	1.00	19.66
ATOM	5803	OH2	TIP	S	59	18.320	33.650	-11.778	1.00	23.35
ATOM	5804	OH2	TIP	S	60	3.811	10.767	-14.624	1.00	21.33
ATOM	5805	OH2	TIP	S	61	10.630	-17.965	40.549	1.00	20.18
ATOM	5806	OH2	TIP	S	62	7.563	12.545	-28.560	1.00	22.05
ATOM	5807	OH2	TIP	S	63	17.504	24.804	2.515	1.00	17.88
ATOM	5808	OH2	TIP	S	64	11.187	4.750	-21.381	1.00	18.39
ATOM	5809	OH2	TIP	S	65	3.669	23.465	0.736	1.00	20.78
ATOM	5810	OH2	TIP	S	66	0.642	-25.439	24.271	1.00	19.92
ATOM	5811	OH2	TIP	S	67	-5.697	-28.454	21.972	1.00	20.88
ATOM	5812	OH2	TIP	S	68	4.514	12.181	-28.340	1.00	18.14
ATOM	5813	OH2	TIP	S	69	-20.340	-23.019	19.925	1.00	21.76
ATOM	5814	OH2	TIP	S	70	1.000	-3.521	35.944	1.00	23.02
ATOM	5815	OH2	TIP	S	71	4.561	34.315	-12.922	1.00	19.38
ATOM	5816	OH2	TIP	S	72	-20.556	2.785	-36.420	1.00	27.46
ATOM	5817	OH2	TIP	S	73	4.764	-1.117	-32.012	1.00	27.35
ATOM	5818	OH2	TIP	S	74	-20.786	-26.799	16.978	1.00	21.37
ATOM	5819	OH2	TIP	S	75	30.429	23.473	16.248	1.00	26.87
ATOM	5820	OH2	TIP	S	76	-14.593	15.544	-36.291	1.00	26.66
ATOM	5821	OH2	TIP	S	77	27.307	15.098	1.258	1.00	25.86
ATOM	5822	OH2	TIP	S	78	5.319	7.976	-32.697	1.00	23.44
ATOM	5823	OH2	TIP	S	79	8.457	-24.862	15.056	1.00	27.61
ATOM	5824	OH2	TIP	S	80	-0.400	-9.335	16.470	1.00	23.64
ATOM	5825	OH2	TIP	S	81	-30.824	-24.685	-8.816	1.00	23.87
ATOM	5826	OH2	TIP	S	82	-2.412	16.657	-12.786	1.00	22.67
ATOM	5827	OH2	TIP	S	83	-16.348	5.876	-33.518	1.00	20.01
ATOM	5828	OH2	TIP	S	84	-4.781	13.922	-43.086	1.00	19.96
ATOM	5829	OH2	TIP	S	85	22.867	14.713	-4.352	1.00	27.67
ATOM	5830	OH2	TIP	S	86	14.019	34.958	-17.016	1.00	24.03
ATOM	5831	OH2	TIP	S	87	-22.863	-7.339	-7.089	1.00	30.51
ATOM	5832	OH2	TIP	S	88	0.014	-13.197	13.132	1.00	24.07
ATOM	5833	OH2	TIP	S	89	-0.477	-26.421	26.641	1.00	22.63
ATOM	5834	OH2	TIP	S	90	8.749	0.467	15.868	1.00	29.65
ATOM	5835	OH2	TIP	S	91	-6.197	-6.594	19.747	1.00	23.37
ATOM	5836	OH2	TIP	S	92	7.703	5.467	-24.148	1.00	20.70
ATOM	5837	OH2	TIP	S	93	1.486	-22.220	27.625	1.00	23.06
ATOM	5838	OH2	TIP	S	94	-8.748	-9.800	20.699	1.00	22.04
ATOM	5839	OH2	TIP	S	95	-16.624	1.189	-13.898	1.00	21.62
ATOM	5840	OH2	TIP	S	96	-17.781	-3.404	-34.492	1.00	24.71
ATOM	5841	OH2	TIP	S	97	22.028	14.095	-22.382	1.00	22.02
ATOM	5842	OH2	TIP	S	98	0.850	24.987	-25.136	1.00	29.29
ATOM	5843	OH2	TIP	S	99	3.761	-8.089	41.138	1.00	24.22
ATOM	5844	OH2	TIP	S	100	6.060	-19.622	23.723	1.00	20.71
ATOM	5845	OH2	TIP	S	101	-20.830	-8.439	-5.124	1.00	25.02
ATOM	5846	OH2	TIP	S	102	-23.978	-22.857	-27.649	1.00	27.37
ATOM	5847	OH2	TIP	S	103	-19.110	-26.350	4.119	1.00	28.04
ATOM	5848	OH2	TIP	S	104	-10.419	10.168	-16.512	1.00	20.89
ATOM	5849	OH2	TIP	S	105	26.620	6.278	5.868	1.00	26.84
ATOM	5850	OH2	TIP	S	106	15.079	-16.710	41.044	1.00	21.49
ATOM	5851	OH2	TIP	S	107	-6.608	-4.481	27.748	1.00	21.60
ATOM	5852	OH2	TIP	S	108	-10.514	-6.785	27.903	1.00	28.76
ATOM	5853	OH2	TIP	S	109	7.483	34.057	-13.520	1.00	20.71
ATOM	5854	OH2	TIP	S	110	-6.501	-31.759	-5.806	1.00	31.23
ATOM	5855	OH2	TIP	S	111	-2.508	-7.957	17.238	1.00	28.35
ATOM	5856	OH2	TIP	S	112	-16.554	3.360	-34.120	1.00	19.83
ATOM	5857	OH2	TIP	S	113	-1.472	10.711	-15.764	1.00	27.87
ATOM	5858	OH2	TIP	S	114	-22.960	-28.887	-19.727	1.00	25.60
ATOM	5859	OH2	TIP	S	115	15.115	-14.901	19.731	1.00	24.51
ATOM	5860	OH2	TIP	S	116	-5.148	-33.100	-3.606	1.00	25.41
ATOM	5861	OH2	TIP	S	117	20.099	-0.396	23.402	1.00	22.68
ATOM	5862	OH2	TIP	S	118	-7.111	-2.117	-16.703	1.00	24.27
ATOM	5863	OH2	TIP	S	119	-11.193	-9.224	19.755	1.00	25.30
ATOM	5864	OH2	TIP	S	120	18.193	-11.449	36.973	1.00	27.57
ATOM	5865	OH2	TIP	S	121	-22.357	2.771	-13.647	1.00	25.49

Figure 1 (continued 59)

ATOM	5866	OH2	TIP	S	123	20.077	32.381	13.831	1.00	28.68
ATOM	5867	OH2	TIP	S	124	-17.741	4.784	-15.367	1.00	27.89
ATOM	5868	OH2	TIP	S	125	4.106	-14.005	15.492	1.00	25.37
ATOM	5869	OH2	TIP	S	126	13.838	16.125	-26.991	1.00	25.20
ATOM	5870	OH2	TIP	S	127	-2.287	-34.498	8.522	1.00	26.09
ATOM	5871	OH2	TIP	S	128	-11.663	-6.092	22.298	1.00	28.13
ATOM	5872	OH2	TIP	S	129	11.561	18.821	-28.755	1.00	36.46
ATOM	5873	OH2	TIP	S	130	7.031	1.863	-26.963	1.00	26.76
ATOM	5874	OH2	TIP	S	131	6.205	-28.726	8.902	1.00	29.30
ATOM	5875	OH2	TIP	S	132	-10.559	19.568	-19.983	1.00	20.77
ATOM	5876	OH2	TIP	S	133	22.972	19.220	-17.034	1.00	20.45
ATOM	5877	OH2	TIP	S	134	5.249	21.787	8.628	1.00	29.10
ATOM	5878	OH2	TIP	S	135	16.410	14.232	27.045	1.00	27.03
ATOM	5879	OH2	TIP	S	136	-3.218	-34.687	11.046	1.00	24.07
ATOM	5880	OH2	TIP	S	137	24.833	28.261	-21.884	1.00	22.96
ATOM	5881	OH2	TIP	S	138	13.264	35.476	-14.774	1.00	30.23
ATOM	5882	OH2	TIP	S	139	-2.053	2.392	26.549	1.00	25.03
ATOM	5883	OH2	TIP	S	140	11.605	15.067	0.133	1.00	34.22
ATOM	5884	OH2	TIP	S	141	13.972	24.010	19.832	1.00	25.81
ATOM	5885	OH2	TIP	S	142	-19.355	-25.503	19.026	1.00	29.46
ATOM	5886	OH2	TIP	S	143	-4.006	-31.965	2.763	1.00	26.41
ATOM	5887	OH2	TIP	S	144	15.901	28.652	-2.514	1.00	25.23
ATOM	5888	OH2	TIP	S	145	-17.355	-32.497	18.572	1.00	25.07
ATOM	5889	OH2	TIP	S	146	0.958	-13.688	32.466	1.00	22.13
ATOM	5890	OH2	TIP	S	147	-6.459	12.128	-44.255	1.00	32.10
ATOM	5891	OH2	TIP	S	148	-0.707	-24.653	2.977	1.00	26.54
ATOM	5892	OH2	TIP	S	149	-12.838	-12.951	11.427	1.00	23.90
ATOM	5893	OH2	TIP	S	150	-24.404	-11.780	-24.495	1.00	25.54
ATOM	5894	OH2	TIP	S	151	0.539	-6.289	-33.601	1.00	29.88
ATOM	5895	OH2	TIP	S	152	-13.161	-28.396	-0.606	1.00	27.46
ATOM	5896	OH2	TIP	S	153	10.877	9.824	5.701	1.00	24.98
ATOM	5897	OH2	TIP	S	154	-24.429	-25.832	1.552	1.00	29.48
ATOM	5898	OH2	TIP	S	155	9.976	29.261	3.159	1.00	26.39
ATOM	5899	OH2	TIP	S	156	-8.594	-7.245	-13.161	1.00	38.12
ATOM	5900	OH2	TIP	S	157	2.066	24.920	5.025	1.00	22.77
ATOM	5901	OH2	TIP	S	158	-15.909	14.296	-28.353	1.00	25.22
ATOM	5902	OH2	TIP	S	159	0.091	16.467	-11.319	1.00	24.31
ATOM	5903	OH2	TIP	S	160	16.526	-12.797	18.583	1.00	26.81
ATOM	5904	OH2	TIP	S	161	3.049	7.864	19.831	1.00	24.57
ATOM	5905	OH2	TIP	S	162	21.865	-8.253	21.271	1.00	23.66
ATOM	5906	OH2	TIP	S	163	-7.960	-6.892	-33.834	1.00	30.32
ATOM	5907	OH2	TIP	S	164	19.362	-16.854	36.055	1.00	31.05
ATOM	5908	OH2	TIP	S	165	-5.308	-32.390	18.952	1.00	29.57
ATOM	5909	OH2	TIP	S	166	-11.933	-29.026	-5.229	1.00	26.58
ATOM	5910	OH2	TIP	S	167	-19.093	-31.089	17.480	1.00	33.54
ATOM	5911	OH2	TIP	S	168	14.092	18.448	-25.956	1.00	29.46
ATOM	5912	OH2	TIP	S	169	10.876	5.438	12.054	1.00	32.82
ATOM	5913	OH2	TIP	S	170	-6.890	-9.072	-26.532	1.00	25.82
ATOM	5914	OH2	TIP	S	171	29.867	28.203	18.182	1.00	30.29
ATOM	5915	OH2	TIP	S	172	16.406	39.004	9.209	1.00	28.96
ATOM	5916	OH2	TIP	S	173	-4.013	-11.245	30.748	1.00	25.90
ATOM	5917	OH2	TIP	S	174	-26.979	-31.890	-8.368	1.00	36.88
ATOM	5918	OH2	TIP	S	175	-23.390	1.597	-33.916	1.00	36.95
ATOM	5919	OH2	TIP	S	176	-21.827	-20.068	21.374	1.00	28.64
ATOM	5920	OH2	TIP	S	177	-17.123	-16.612	7.118	1.00	25.01
ATOM	5921	OH2	TIP	S	178	-0.586	30.510	-11.769	1.00	23.24
ATOM	5922	OH2	TIP	S	179	6.159	20.259	17.337	1.00	30.73
ATOM	5923	OH2	TIP	S	180	21.260	-1.762	19.163	1.00	34.09
ATOM	5924	OH2	TIP	S	181	-2.864	-28.282	2.753	1.00	27.53
ATOM	5925	OH2	TIP	S	182	-8.835	-11.179	-6.743	1.00	29.61
ATOM	5926	OH2	TIP	S	183	15.829	24.884	-23.368	1.00	31.33
ATOM	5927	OH2	TIP	S	184	24.002	17.831	-10.733	1.00	29.65
ATOM	5928	OH2	TIP	S	185	-29.401	5.440	-14.949	1.00	32.48
ATOM	5929	OH2	TIP	S	186	-1.383	-33.459	19.317	1.00	29.25
ATOM	5930	OH2	TIP	S	187	12.063	-19.966	25.080	1.00	25.65
ATOM	5931	OH2	TIP	S	188	-4.351	-9.679	-26.788	1.00	27.17
ATOM	5932	OH2	TIP	S	189	3.729	5.832	16.486	1.00	34.24
ATOM	5933	OH2	TIP	S	190	9.565	37.434	-9.975	1.00	27.30
ATOM	5934	OH2	TIP	S	191	1.483	14.975	-40.508	1.00	31.36
ATOM	5935	OH2	TIP	S	192	-6.648	-10.961	-20.165	1.00	32.28
ATOM	5936	OH2	TIP	S	193	3.745	12.221	31.113	1.00	29.48
ATOM	5937	OH2	TIP	S	194	2.400	-29.701	-15.849	1.00	26.51
ATOM	5938	OH2	TIP	S	195	1.145	-29.287	18.977	1.00	27.97
ATOM	5939	OH2	TIP	S	196	1.173	24.321	-30.127	1.00	37.69
ATOM	5940	OH2	TIP	S	197	-28.254	-20.580	5.716	1.00	43.95
ATOM	5941	OH2	TIP	S	198	22.283	20.039	25.715	1.00	34.76
ATOM	5942	OH2	TIP	S	199	-1.895	4.664	-43.775	1.00	27.75
ATOM	5943	OH2	TIP	S	200	23.429	31.198	-15.860	1.00	32.99
ATOM	5944	OH2	TIP	S	201	-9.479	-5.901	-15.419	1.00	21.16
ATOM	5945	OH2	TIP	S	202	-12.878	0.162	-12.723	1.00	33.84
ATOM	5946	OH2	TIP	S	203	5.581	19.187	14.793	1.00	27.97
ATOM	5947	OH2	TIP	S	204	-23.954	-24.578	-2.262	1.00	30.51
ATOM	5948	OH2	TIP	S	205	3.457	33.211	-23.268	1.00	31.98
ATOM	5949	OH2	TIP	S	206	-17.263	0.457	-42.268	1.00	31.49
ATOM	5950	OH2	TIP	S	207	16.260	31.888	2.413	1.00	23.24
ATOM	5951	OH2	TIP	S	208	-4.320	1.145	26.565	1.00	29.38
ATOM	5952	OH2	TIP	S	209	-19.947	2.160	-11.744	1.00	38.41
ATOM	5953	OH2	TIP	S	210	1.872	26.689	-27.041	1.00	29.78
ATOM	5954	OH2	TIP	S	211	-13.714	23.099	-13.845	1.00	33.77
ATOM	5955	OH2	TIP	S	212	9.218	35.580	-19.331	1.00	29.22
ATOM	5956	OH2	TIP	S	213	-0.219	26.259	5.173	1.00	31.76
ATOM	5957	OH2	TIP	S	214	-8.272	3.938	-13.966	1.00	35.25
ATOM	5958	OH2	TIP	S	215	9.984	-22.548	31.867	1.00	33.85
ATOM	5959	OH2	TIP	S	216	-30.386	-28.425	2.476	1.00	30.05
ATOM	5960	OH2	TIP	S	217	5.272	16.545	-36.105	1.00	33.30
ATOM	5961	OH2	TIP	S	218	-14.957	-2.170	-39.231	1.00	30.96
ATOM	5962	OH2	TIP	S	219	2.136	-28.546	23.097	1.00	39.83
ATOM	5963	OH2	TIP	S	220	0.866	11.873	23.871	1.00	32.14
ATOM	5964	OH2	TIP	S	221	-7.469	-8.003	-23.367	1.00	24.79
ATOM	5965	OH2	TIP	S	222	10.219	6.251	34.646	1.00	37.06

Figure 1 (continued 60)

ATOM	5966	OH2	TIP	S	223	9.603	-19.191	12.099	1.00	30.03
ATOM	5967	OH2	TIP	S	224	15.592	1.270	14.898	1.00	29.33
ATOM	5968	OH2	TIP	S	225	-7.625	-22.611	-22.802	1.00	32.63
ATOM	5969	OH2	TIP	S	226	-30.236	-24.968	-11.543	1.00	24.51
ATOM	5970	OH2	TIP	S	227	-11.748	-27.136	28.999	1.00	35.80
ATOM	5971	OH2	TIP	S	228	-17.912	-19.364	23.072	1.00	31.69
ATOM	5972	OH2	TIP	S	229	-12.001	4.279	-15.335	1.00	28.59
ATOM	5973	OH2	TIP	S	230	27.573	31.316	11.831	1.00	32.14
ATOM	5974	OH2	TIP	S	231	-25.350	3.037	-21.957	1.00	30.50
ATOM	5975	OH2	TIP	S	232	-9.948	19.698	-27.138	1.00	32.26
ATOM	5976	OH2	TIP	S	233	31.351	11.309	12.566	1.00	40.60
ATOM	5977	OH2	TIP	S	234	7.345	8.147	-8.973	1.00	40.15
ATOM	5978	OH2	TIP	S	235	13.323	25.650	-24.378	1.00	28.39
ATOM	5979	OH2	TIP	S	236	14.326	-23.002	38.347	1.00	44.20
ATOM	5980	OH2	TIP	S	237	18.205	35.226	-19.376	1.00	36.69
ATOM	5981	OH2	TIP	S	238	7.073	7.343	-21.458	1.00	26.18
ATOM	5982	OH2	TIP	S	239	6.134	-17.380	11.852	1.00	34.32
ATOM	5983	OH2	TIP	S	240	-6.807	3.536	-42.001	1.00	25.28
ATOM	5984	OH2	TIP	S	241	-24.937	-17.863	-25.603	1.00	32.04
ATOM	5985	OH2	TIP	S	242	-17.088	-21.664	-30.797	1.00	30.50
ATOM	5986	OH2	TIP	S	243	6.771	-7.663	14.406	1.00	36.01
ATOM	5987	OH2	TIP	S	244	-27.706	-30.578	-5.708	1.00	47.96
ATOM	5988	OH2	TIP	S	245	-21.059	10.316	-25.562	1.00	35.65
ATOM	5989	OH2	TIP	S	246	10.606	28.216	-25.525	1.00	29.43
ATOM	5990	OH2	TIP	S	247	1.528	5.171	-17.593	1.00	27.85
ATOM	5991	OH2	TIP	S	248	-29.012	-18.667	-20.134	1.00	33.27
ATOM	5992	OH2	TIP	S	249	-21.413	-24.799	4.888	1.00	34.44
ATOM	5993	OH2	TIP	S	250	1.196	-8.297	-29.245	1.00	27.57
ATOM	5994	OH2	TIP	S	251	-0.162	-13.772	35.108	1.00	36.60
ATOM	5995	OH2	TIP	S	252	19.156	-15.454	21.696	1.00	29.04
ATOM	5996	OH2	TIP	S	253	21.723	17.101	-18.745	1.00	9.13
ATOM	5997	OH2	TIP	S	254	7.667	9.573	-26.321	1.00	15.05
ATOM	5998	OH2	TIP	S	255	5.459	9.537	-28.155	1.00	14.20
ATOM	5999	OH2	TIP	S	256	7.583	-20.372	19.535	1.00	17.45
ATOM	6000	OH2	TIP	S	257	8.434	5.091	-21.601	1.00	20.19
ATOM	6001	OH2	TIP	S	258	10.303	-20.727	39.479	1.00	21.19
ATOM	6002	OH2	TIP	S	259	23.351	15.777	-20.932	1.00	24.25
ATOM	6003	OH2	TIP	S	260	8.255	-19.223	21.937	1.00	16.91
ATOM	6004	OH2	TIP	S	261	7.407	21.555	-29.683	1.00	18.42
ATOM	6005	OH2	TIP	S	262	0.133	-33.614	9.571	1.00	23.67
ATOM	6006	OH2	TIP	S	263	1.067	23.311	-27.412	1.00	26.04
ATOM	6007	OH2	TIP	S	264	10.172	-20.657	23.070	1.00	20.75
ATOM	6008	OH2	TIP	S	265	5.434	1.347	-31.078	1.00	25.19
ATOM	6009	OH2	TIP	S	266	6.473	8.791	-30.462	1.00	22.73
ATOM	6010	OH2	TIP	S	267	16.690	-16.534	21.428	1.00	23.86
ATOM	6011	OH2	TIP	S	268	-7.886	21.056	-13.245	1.00	26.88
ATOM	6012	OH2	TIP	S	269	12.771	20.121	-27.176	1.00	33.96
ATOM	6013	OH2	TIP	S	270	-17.226	9.655	-21.614	1.00	26.62
ATOM	6014	OH2	TIP	S	271	-2.213	14.948	-43.167	1.00	24.56
ATOM	6015	OH2	TIP	S	272	9.664	5.525	-25.968	1.00	25.69
ATOM	6016	OH2	TIP	S	273	6.917	-25.402	17.512	1.00	27.80
ATOM	6017	OH2	TIP	S	274	-4.242	-20.885	28.965	1.00	32.23
ATOM	6018	OH2	TIP	S	275	-17.221	-17.062	17.975	1.00	28.09
ATOM	6019	OH2	TIP	S	276	12.668	11.417	-26.228	1.00	27.75
ATOM	6020	OH2	TIP	S	277	10.299	1.950	14.305	1.00	27.65
ATOM	6021	OH2	TIP	S	278	-31.806	-30.359	-6.948	1.00	57.47
ATOM	6022	OH2	TIP	S	279	-26.463	4.339	-9.507	1.00	29.65
ATOM	6023	OH2	TIP	S	280	-26.015	-34.574	7.677	1.00	26.06
ATOM	6024	OH2	TIP	S	281	-31.347	5.379	-17.218	1.00	33.42
ATOM	6025	OH2	TIP	S	282	14.453	-16.744	17.668	1.00	30.41
ATOM	6026	OH2	TIP	S	283	27.710	8.976	5.055	1.00	26.81
ATOM	6027	OH2	TIP	S	284	2.896	8.795	-16.720	1.00	27.99
ATOM	6028	OH2	TIP	S	285	-9.100	19.482	-24.203	1.00	25.80
ATOM	6029	OH2	TIP	S	286	-2.579	1.667	21.500	1.00	29.60
ATOM	6030	OH2	TIP	S	287	6.335	11.378	-31.555	1.00	29.71
ATOM	6031	OH2	TIP	S	288	12.371	-16.564	41.802	1.00	31.26
ATOM	6032	OH2	TIP	S	289	0.360	-29.275	21.468	1.00	31.50
ATOM	6033	OH2	TIP	S	290	-2.645	4.725	26.240	1.00	33.72
ATOM	6034	OH2	TIP	S	291	19.718	-0.267	20.338	1.00	32.39
ATOM	6035	OH2	TIP	S	292	7.034	29.199	9.979	1.00	29.78
ATOM	6036	OH2	TIP	S	293	-4.995	20.991	-12.507	1.00	34.58
ATOM	6037	OH2	TIP	S	294	-28.086	-24.068	-26.481	1.00	30.52
ATOM	6038	OH2	TIP	S	295	4.690	32.380	-25.768	1.00	32.16
ATOM	6039	OH2	TIP	S	296	12.183	37.736	-9.852	1.00	32.44
ATOM	6040	OH2	TIP	S	297	-0.897	-9.935	-28.834	1.00	28.74
ATOM	6041	OH2	TIP	S	298	-5.666	-26.946	-3.776	1.00	35.30
ATOM	6042	OH2	TIP	S	299	-19.121	-17.609	23.997	1.00	30.20
ATOM	6043	OH2	TIP	S	300	11.846	2.521	-20.488	1.00	34.76
ATOM	6044	OH2	TIP	S	301	21.299	6.735	24.995	1.00	37.00
ATOM	6045	OH2	TIP	S	302	-23.638	-27.161	16.432	1.00	29.19
ATOM	6046	OH2	TIP	S	303	1.556	-0.845	-22.820	1.00	34.60
ATOM	6047	OH2	TIP	S	304	-12.057	-30.800	-2.592	1.00	30.84
ATOM	6048	OH2	TIP	S	305	16.694	-19.967	30.452	1.00	32.66
ATOM	6049	OH2	TIP	S	306	0.157	25.634	-7.191	1.00	32.17
ATOM	6050	OH2	TIP	S	307	-0.449	27.840	-20.073	1.00	29.18
ATOM	6051	OH2	TIP	S	308	21.819	3.025	9.910	1.00	41.68
ATOM	6052	OH2	TIP	S	309	-15.005	-11.439	-28.535	1.00	38.02
ATOM	6053	OH2	TIP	S	310	-21.942	-31.716	-8.240	1.00	33.01
ATOM	6054	OH2	TIP	S	311	-8.284	-25.125	-23.593	1.00	41.18
ATOM	6055	OH2	TIP	S	312	2.515	4.002	-33.125	1.00	26.47
ATOM	6056	OH2	TIP	S	313	-18.335	13.849	-29.235	1.00	30.43
ATOM	6057	OH2	TIP	S	314	-12.912	-8.449	21.566	1.00	30.42
ATOM	6058	OH2	TIP	S	315	-1.397	-26.362	1.310	1.00	33.91
ATOM	6059	OH2	TIP	S	316	9.366	-22.526	35.732	1.00	30.66
ATOM	6060	OH2	TIP	S	317	-25.401	-30.023	-8.998	1.00	29.44
ATOM	6061	OH2	TIP	S	318	-21.887	3.702	-34.234	1.00	36.98
ATOM	6062	OH2	TIP	S	319	-8.700	-20.782	-24.886	1.00	32.89
ATOM	6063	OH2	TIP	S	320	-20.333	-29.925	-6.872	1.00	34.64
ATOM	6064	OH2	TIP	S	321	-7.827	-13.241	-33.387	1.00	32.71
ATOM	6065	OH2	TIP	S	322	14.750	31.182	9.293	1.00	31.66

Figure 1 (continued 61)

ATOM	6066	OH2	TIP	S	323	-24.400	-19.167	20.554	1.00	30.46
ATOM	6067	OH2	TIP	S	324	-9.584	3.692	-42.248	1.00	33.30
ATOM	6068	OH2	TIP	S	325	6.014	19.032	-31.179	1.00	40.38
ATOM	6069	OH2	TIP	S	326	-13.974	-30.622	-5.965	1.00	32.26
ATOM	6070	OH2	TIP	S	327	-29.857	-10.593	-7.579	1.00	34.80
ATOM	6071	OH2	TIP	S	328	12.690	33.497	-20.379	1.00	34.07
ATOM	6072	OH2	TIP	S	329	7.069	2.658	-20.988	1.00	28.88
ATOM	6073	OH2	TIP	S	330	12.019	-0.360	36.086	1.00	26.34
ATOM	6074	OH2	TIP	S	331	-22.705	5.938	-14.330	1.00	34.70
ATOM	6075	OH2	TIP	S	332	8.097	14.122	-2.649	1.00	39.46
ATOM	6076	OH2	TIP	S	333	-21.898	-21.927	4.044	1.00	37.81
ATOM	6077	OH2	TIP	S	334	9.937	-17.771	16.216	1.00	29.70
ATOM	6078	OH2	TIP	S	335	-16.221	-6.845	-33.678	1.00	33.31
ATOM	6079	OH2	TIP	S	336	-3.494	-22.898	-17.063	1.00	31.83
ATOM	6080	OH2	TIP	S	337	-22.157	5.573	-30.240	1.00	39.35
ATOM	6081	OH2	TIP	S	338	-7.617	-32.398	-8.188	1.00	30.34
ATOM	6082	OH2	TIP	S	339	23.475	29.150	-8.430	1.00	36.32
ATOM	6083	OH2	TIP	S	340	-7.276	-9.187	-35.186	1.00	41.69
ATOM	6084	OH2	TIP	S	341	26.845	32.870	8.481	1.00	37.63
ATOM	6085	OH2	TIP	S	342	-12.192	21.236	-21.321	1.00	30.21
ATOM	6086	OH2	TIP	S	343	-14.628	-35.461	19.832	1.00	35.16
ATOM	6087	OH2	TIP	S	344	-5.653	-31.128	21.101	1.00	34.25
ATOM	6088	OH2	TIP	S	345	-6.084	-8.172	-19.496	1.00	36.21
ATOM	6089	OH2	TIP	S	346	27.089	28.347	6.056	1.00	42.19
ATOM	6090	OH2	TIP	S	347	17.043	22.284	-26.012	1.00	32.12
ATOM	6091	OH2	TIP	S	348	-21.277	2.842	-26.424	1.00	36.86
ATOM	6092	OH2	TIP	S	349	-23.886	-14.574	-31.320	1.00	39.26
ATOM	6093	OH2	TIP	S	350	5.980	19.532	10.965	1.00	26.13
ATOM	6094	OH2	TIP	S	351	15.574	-9.666	16.201	1.00	35.41
ATOM	6095	OH2	TIP	S	352	-20.467	-13.308	-4.732	1.00	35.05
ATOM	6096	OH2	TIP	S	353	3.368	14.285	32.732	1.00	36.22
ATOM	6097	OH2	TIP	S	354	-7.181	18.881	-31.723	1.00	38.24
ATOM	6098	OH2	TIP	S	355	-28.089	-22.839	-28.744	1.00	37.10
ATOM	6099	OH2	TIP	S	356	20.976	15.824	-10.655	1.00	30.49
ATOM	6100	OH2	TIP	S	357	-28.758	-11.680	-18.762	1.00	43.84
ATOM	6101	OH2	TIP	S	358	7.259	27.237	24.216	1.00	31.98
ATOM	6102	OH2	TIP	S	359	-1.640	22.549	-9.537	1.00	38.37
ATOM	6103	OH2	TIP	S	360	-4.918	-24.935	-15.685	1.00	33.12
ATOM	6104	OH2	TIP	S	361	4.941	-2.575	16.309	1.00	34.53
ATOM	6105	OH2	TIP	S	362	9.096	-17.304	13.805	1.00	34.10
ATOM	6106	OH2	TIP	S	363	-5.045	-8.870	15.785	1.00	31.53
ATOM	6107	OH2	TIP	S	364	17.874	2.521	14.615	1.00	34.86
ATOM	6108	OH2	TIP	S	365	-10.159	-16.244	-28.446	1.00	36.25
ATOM	6109	OH2	TIP	S	366	4.946	7.818	-15.134	1.00	34.00
ATOM	6110	OH2	TIP	S	367	-6.685	-11.153	14.460	1.00	40.57
ATOM	6111	OH2	TIP	S	368	14.487	-20.336	24.009	1.00	34.28
ATOM	6112	OH2	TIP	S	369	-1.563	6.524	-45.958	1.00	39.83
ATOM	6113	OH2	TIP	S	370	0.375	7.077	23.000	1.00	42.33
ATOM	6114	OH2	TIP	S	371	17.591	31.139	0.347	1.00	41.73
ATOM	6115	OH2	TIP	S	372	-16.867	13.392	-37.376	1.00	41.23
ATOM	6116	OH2	TIP	S	373	-12.567	7.824	-44.159	1.00	31.69
ATOM	6117	OH2	TIP	S	374	26.381	23.140	-10.721	1.00	40.85
ATOM	6118	OH2	TIP	S	375	9.272	35.080	2.703	1.00	40.96
ATOM	6119	OH2	TIP	S	376	9.264	3.347	41.197	1.00	34.17
ATOM	6120	OH2	TIP	S	377	25.188	14.056	27.610	1.00	42.27
ATOM	6121	OH2	TIP	S	378	5.411	-5.742	41.987	1.00	32.59
ATOM	6122	OH2	TIP	S	379	-11.338	22.385	-17.862	1.00	32.84
ATOM	6123	OH2	TIP	S	380	-20.579	13.226	-28.071	1.00	34.93
ATOM	6124	OH2	TIP	S	381	8.683	9.553	-13.934	1.00	42.23
ATOM	6125	OH2	TIP	S	382	0.828	11.135	-19.564	1.00	35.82
ATOM	6126	OH2	TIP	S	383	-21.600	-31.698	15.485	1.00	31.57
ATOM	6127	OH2	TIP	S	384	21.597	31.274	4.587	1.00	38.64
ATOM	6128	OH2	TIP	S	385	12.268	35.903	-11.527	1.00	40.11
ATOM	6129	OH2	TIP	S	386	-10.826	21.324	-8.086	1.00	31.64
ATOM	6130	OH2	TIP	S	387	20.994	17.489	-26.433	1.00	38.40
ATOM	6131	OH2	TIP	S	388	-18.148	20.285	25.908	1.00	37.68
ATOM	6132	OH2	TIP	S	389	18.469	17.950	-44.136	1.00	37.56
ATOM	6133	OH2	TIP	S	390	-17.756	2.318	18.962	1.00	37.13
ATOM	6134	OH2	TIP	S	391	23.292	-5.751	-24.110	1.00	34.35
ATOM	6135	OH2	TIP	S	392	-5.798	2.354	-15.393	1.00	33.61
ATOM	6136	OH2	TIP	S	393	2.260	-2.829	-16.208	1.00	40.16
ATOM	6137	OH2	TIP	S	394	-1.341	7.648	0.420	1.00	35.70
ATOM	6138	OH2	TIP	S	395	14.575	6.039	24.816	1.00	30.69
ATOM	6139	OH2	TIP	S	396	21.269	15.381	20.987	1.00	38.19
ATOM	6140	OH2	TIP	S	397	11.903	28.956	-5.640	1.00	37.49
ATOM	6141	OH2	TIP	S	398	8.524	-21.963	7.979	1.00	34.27
ATOM	6142	OH2	TIP	S	399	-19.214	-17.096	1.767	1.00	36.13
ATOM	6143	OH2	TIP	S	400	-30.167	-21.541	-1.917	1.00	31.35
ATOM	6144	OH2	TIP	S	401	9.901	9.176	-1.067	1.00	35.17
ATOM	6145	OH2	TIP	S	402	-4.981	-29.566	35.320	1.00	29.07
ATOM	6146	OH2	TIP	S	403	22.136	13.679	23.153	1.00	39.40
ATOM	6147	OH2	TIP	S	404	-13.420	-2.821	-24.806	1.00	31.71
ATOM	6148	OH2	TIP	S	405	-21.015	-10.324	29.465	1.00	39.24
ATOM	6149	OH2	TIP	S	406	4.107	-17.741	-4.370	1.00	38.21
ATOM	6150	OH2	TIP	S	407	20.599	24.525	-26.039	1.00	31.58
ATOM	6151	OH2	TIP	S	408	-29.430	-5.137	-12.054	1.00	42.29
ATOM	6152	OH2	TIP	S	409	5.574	17.571	33.040	1.00	35.29
ATOM	6153	OH2	TIP	S	410	25.806	21.628	19.314	1.00	36.07
ATOM	6154	OH2	TIP	S	411	-18.143	-31.597	-23.592	1.00	38.57
ATOM	6155	OH2	TIP	S	412	-1.328	25.281	18.671	1.00	41.38
ATOM	6156	OH2	TIP	S	413	0.344	10.818	-9.446	1.00	37.29
ATOM	6157	OH2	TIP	S	414	-18.150	-29.804	32.614	1.00	36.54
ATOM	6158	OH2	TIP	S	415	-23.823	-3.528	17.628	1.00	39.18
ATOM	6159	OH2	TIP	S	416	1.739	1.943			
ATOM	6160	OH2	TIP	S	417	-27.131	-17.300			
ATOM	6161	OH2	TIP	S	418	17.275	0.759			
ATOM	6162	OH2	TIP	S	419	0.007	26.223			
ATOM	6163	OH2	TIP	S	420	-13.181	-10.416			
ATOM	6164	OH2	TIP	S	421	-18.110	16.629			
ATOM	6165	OH2	TIP	S	422	7.358	26.526			

Figure 1 (continued 62)

അനുബന്ധം 1

Figure 1 (continued 63)

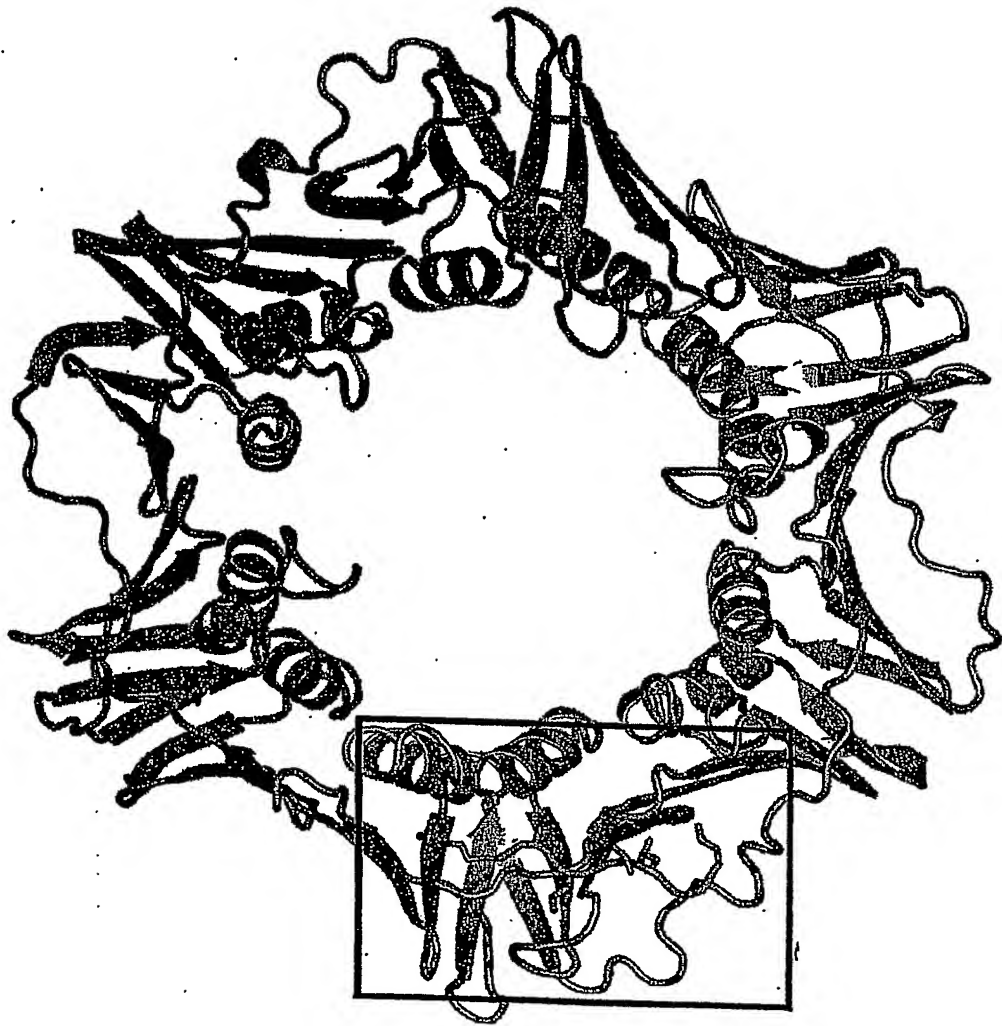


Figure 2

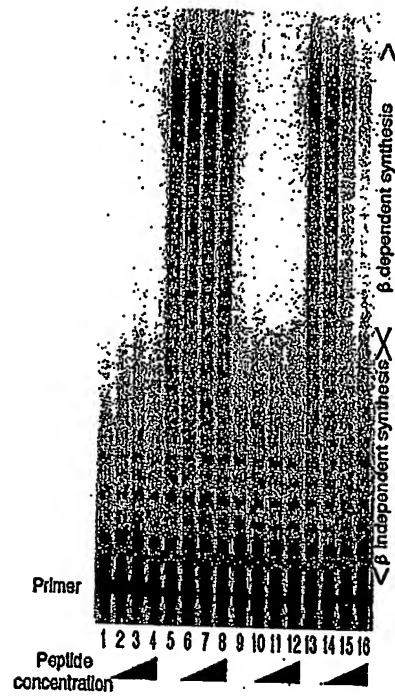


Figure 3A

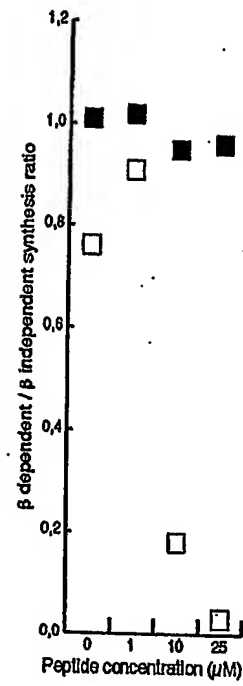


Figure 3B

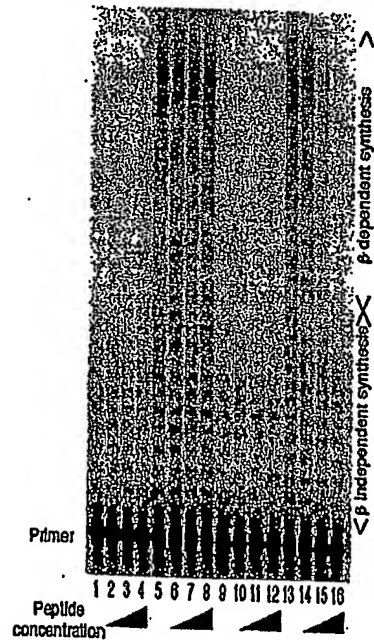


Figure 3C

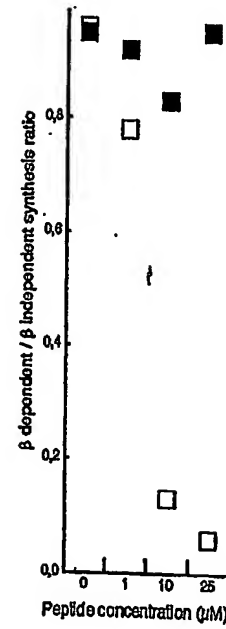


Figure 3D

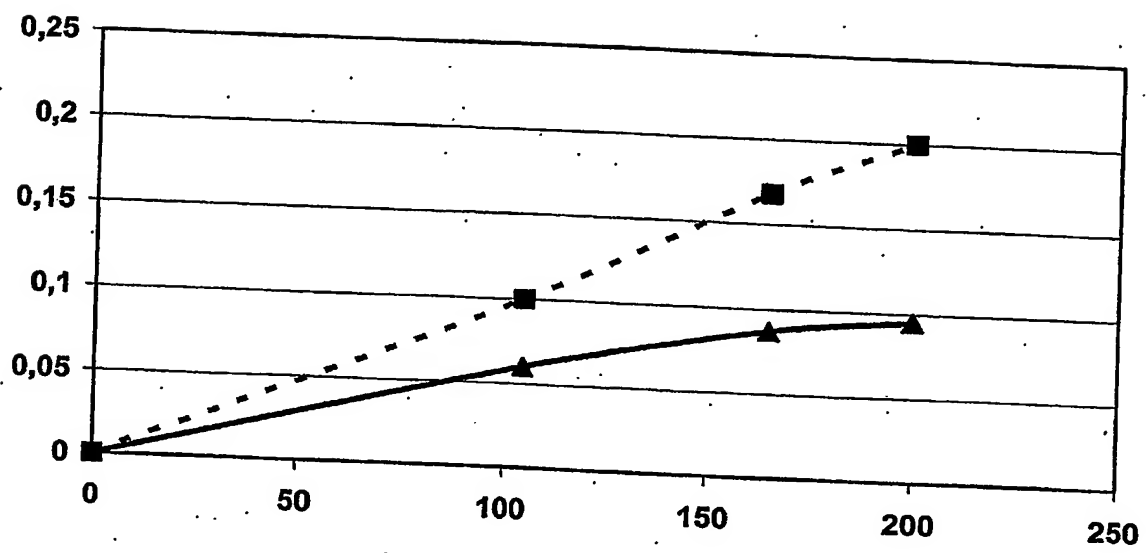


Figure 4

SEQUENCE LISTING

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PCT/EP2004/006942

